Full wwPDB EM Validation Report ⓘ

Nov 7, 2023 – 06:00 am GMT

PDB ID	:	8PV7
EMDB ID	:	EMD-17956
Title	:	Chaetomium thermophilum pre-60S State 1 - pre-5S rotation (Arx1/Nog2 state) - Composite structure
Authors	:	Thoms, M.; Cheng, J.; Denk, T.; Berninghausen, O.; Beckmann, R.
Deposited on	:	2023-07-17
Resolution	:	2.12 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

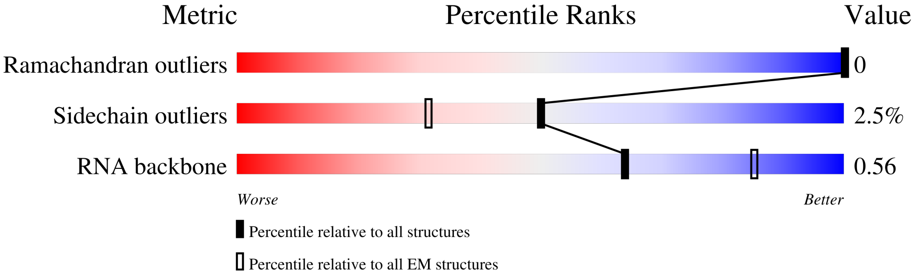
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

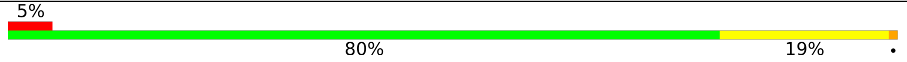
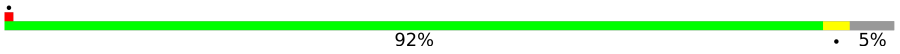
The reported resolution of this entry is 2.12 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C1	3342	
2	C2	156	
3	C3	162	
4	C4	119	
5	CB	391	
6	CF	270	
7	CH	661	
8	CI	414	

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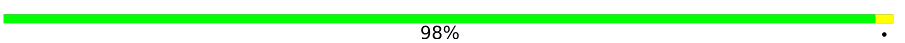
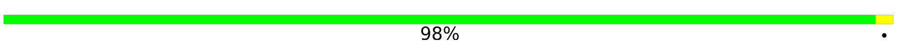
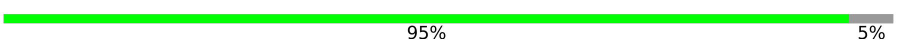
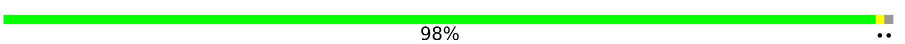
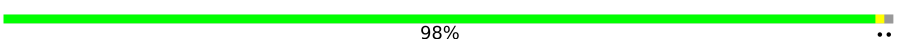
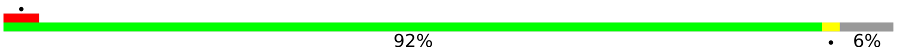
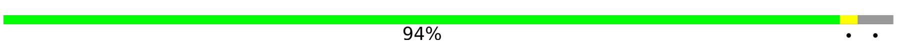
Mol	Chain	Length	Quality of chain
9	CJ	679	
10	CK	261	
11	CL	558	
12	CM	249	
12	LF	249	
13	CN	246	
14	CO	120	
15	CQ	225	
16	Lq	147	
17	Cb	117	
18	Cd	627	
19	Ce	443	
20	Cf	350	
21	Cg	202	
22	Ch	517	
23	Cz	123	
24	LA	254	
25	LB	392	
26	LC	365	
27	LD	304	
28	LE	200	
29	LG	262	
30	LH	229	
31	LJ	173	
32	LK	165	

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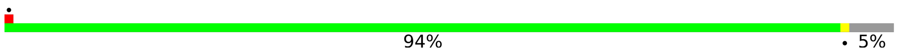
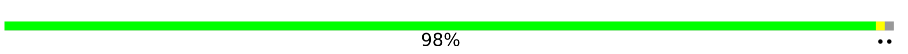
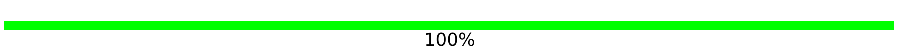
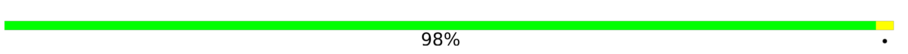
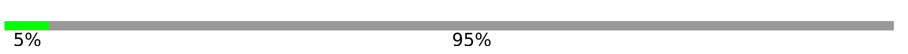
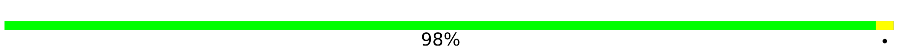
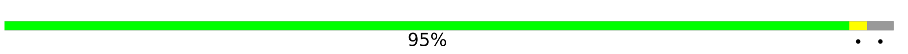
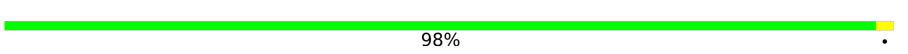
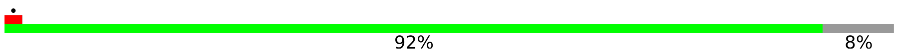
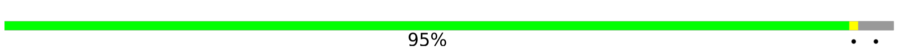
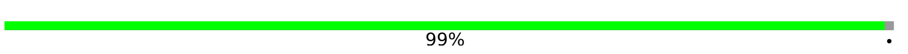
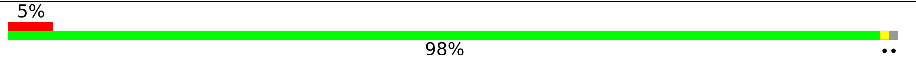
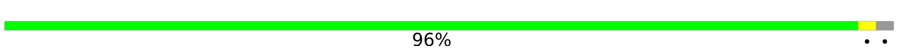
Mol	Chain	Length	Quality of chain
33	LL	213	
34	LM	142	
35	LN	203	
36	LO	204	
37	LP	187	
38	LQ	213	
39	LR	2898	
40	LS	174	
41	LT	160	
42	LU	127	
43	LV	139	
44	LX	156	
45	LY	138	
46	LZ	135	
47	La	149	
48	Lc	108	
49	Ld	120	
50	Le	131	
51	Lf	109	
52	Lg	119	
53	Lh	935	
54	Li	110	
55	Lj	95	
56	Lk	94	
57	Ll	51	

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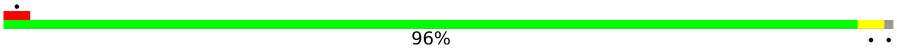
Mol	**Chain**	**Length**	**Quality of chain**
58	Lp	92	

2 Entry composition ⓘ

There are 62 unique types of molecules in this entry. The entry contains 157262 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 26S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	C1	3078	65888	29429	11926	21455	3078	0	0

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	C2	156	3319	1484	589	1090	156	0	0

- Molecule 3 is a RNA chain called ITS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C3	82	1754	780	316	576	82	0	0

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	C4	119	2536	1131	453	833	119	0	0

- Molecule 5 is a protein called Utp30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	CB	267	2119	1359	373	384	3	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	CF	245	1934	1215	350	360	9	0	0

- Molecule 7 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	CH	627	5063	3181	924	939	19	0	0

- Molecule 8 is a protein called Putative RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	CI	152	1234	791	230	208	5	0	0

- Molecule 9 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	CJ	382	3116	2008	548	550	10	0	0

- Molecule 10 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	CK	237	1903	1198	368	333	4	0	0

- Molecule 11 is a protein called Putative GTP binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	CL	79	622	389	125	108	0	0

- Molecule 12 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	CM	217	1773	1144	329	297	3	0	0
12	LF	248	2023	1297	377	346	3	0	0

- Molecule 13 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	CN	246	1853	1156	322	368	7	0	0

- Molecule 14 is a protein called DUF2423 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	CO	62	Total 468	C 290	N 94	O 82	S 2	0	0

- Molecule 15 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	CQ	183	Total 1480	C 925	N 304	O 241	S 10	0	0

- Molecule 16 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Lq	139	Total 1073	C 672	N 213	O 188	0	0

- Molecule 17 is a protein called Zinc finger domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Cb	101	Total 830	C 517	N 161	O 148	S 4	0	0

- Molecule 18 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Cd	462	Total 3691	C 2350	N 671	O 659	S 11	0	0

- Molecule 19 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Ce	262	Total 2148	C 1337	N 413	O 394	S 4	0	0

- Molecule 20 is a protein called Ribosome production factor 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Cf	285	Total 2282	C 1443	N 417	O 401	S 21	0	0

- Molecule 21 is a protein called Ribosome biogenesis regulatory protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Cg	188	1478	924	283	270	1	0	0

- Molecule 22 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Ch	485	3812	2396	696	710	10	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ch	117	ASP	GLU	engineered mutation	UNP G0SC29

- Molecule 23 is a protein called rRNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Cz	101	869	541	180	144	4	0	0

- Molecule 24 is a protein called 60S ribosomal protein L2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	LA	191	1454	917	278	256	3	0	0

- Molecule 25 is a protein called 60S ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	LB	389	3104	1973	579	539	13	0	0

- Molecule 26 is a protein called 60S ribosomal protein L4-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	LC	363	2751	1737	527	478	9	0	0

- Molecule 27 is a protein called 60S ribosomal protein l5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	LD	286	2266	1434	407	422	3	0	0

- Molecule 28 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	LE	191	1477	944	267	263	3	0	0

- Molecule 29 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	LG	235	1889	1210	350	324	5	0	0

- Molecule 30 is a protein called 60S ribosomal protein l9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	LH	190	1495	949	268	272	6	0	0

- Molecule 31 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	LJ	169	1357	850	266	235	6	0	0

- Molecule 32 is a protein called 60S ribosomal protein L12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	LK	158	1184	743	215	224	2	0	0

- Molecule 33 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	LL	203	1587	989	325	271	2	0	0

- Molecule 34 is a protein called 60S ribosomal protein L14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	LM	141	1126	714	216	195	1	0	0

- Molecule 35 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	LN	202	1704	1062	360	278	4	0	0

- Molecule 36 is a protein called 60S ribosomal protein L16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	LO	203	1611	1034	305	267	5	0	0

- Molecule 37 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	LP	171	1343	834	274	232	3	0	0

- Molecule 38 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	LQ	150	1200	759	239	200	2	0	0

- Molecule 39 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	LR	155	1241	772	262	203	4	0	0

- Molecule 40 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	LS	174	1426	917	266	238	5	0	0

- Molecule 41 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	LT	129	1027	651	195	179	2	0	0

- Molecule 42 is a protein called 60S ribosomal protein L22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	LU	105	846	548	146	151	1	0	0

- Molecule 43 is a protein called 60S ribosomal protein l23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	LV	135	991	630	184	170	7	0	0

- Molecule 44 is a protein called 60S ribosomal protein L25-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	LX	145	1133	723	211	199	0	0

- Molecule 45 is a protein called 60S ribosomal protein L26-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	LY	133	1056	658	213	183	2	0	0

- Molecule 46 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	LZ	135	1112	713	207	188	4	0	0

- Molecule 47 is a protein called 60S ribosomal protein L28-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	La	108	872	556	168	147	1	0	0

- Molecule 48 is a protein called 60S ribosomal protein l30-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Lc	95	Total 705	C 449	N 122	O 129	S 5	0	0

- Molecule 49 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Ld	110	Total 875	C 555	N 171	O 148	S 1	0	0

- Molecule 50 is a protein called 60S ribosomal protein L32-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Le	126	Total 1017	C 640	N 208	O 163	S 6	0	0

- Molecule 51 is a protein called 60S ribosomal protein l33-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Lf	108	Total 862	C 546	N 171	O 144	S 1	0	0

- Molecule 52 is a protein called Ribosomal protein l34-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Lg	118	Total 914	C 567	N 186	O 157	S 4	0	0

- Molecule 53 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	Lh	122	Total 1003	C 637	N 198	O 168	0	0

- Molecule 54 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Li	101	Total 827	C 509	N 181	O 136	S 1	0	0

- Molecule 55 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	Lj	88	698	427	154	112	5	0	0

- Molecule 56 is a protein called 60S ribosomal protein L38-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	Lk	76	632	400	121	109	2	0	0

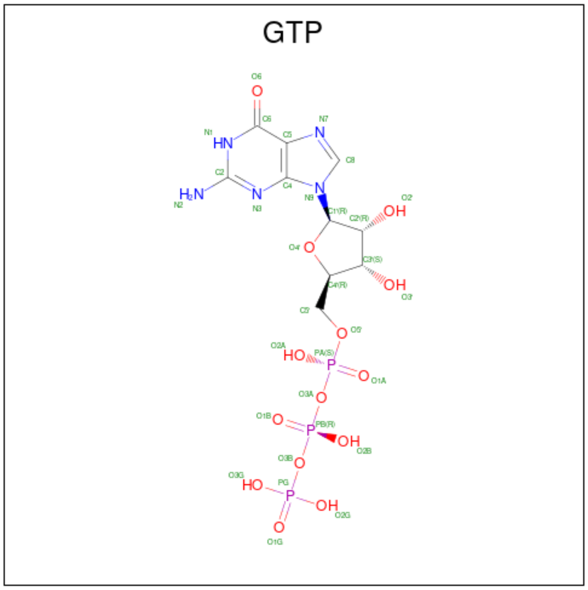
- Molecule 57 is a protein called Ribosomal protein eL39.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
57	Ll	50	436	275	97	64	0	0

- Molecule 58 is a protein called 60S ribosomal protein L43-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	Lp	91	698	430	138	124	6	0	0

- Molecule 59 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
59	CH	1	32	10	5	14	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
59	Cd	1	Total 32	C 10	N 5	O 14	P 3	0

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	CH	1	Total 1	Mg 1	0
60	Cd	2	Total 2	Mg 2	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	CQ	1	Total 1	Zn 1	0
61	Cb	1	Total 1	Zn 1	0
61	Lg	1	Total 1	Zn 1	0
61	Lj	1	Total 1	Zn 1	0
61	Lp	1	Total 1	Zn 1	0

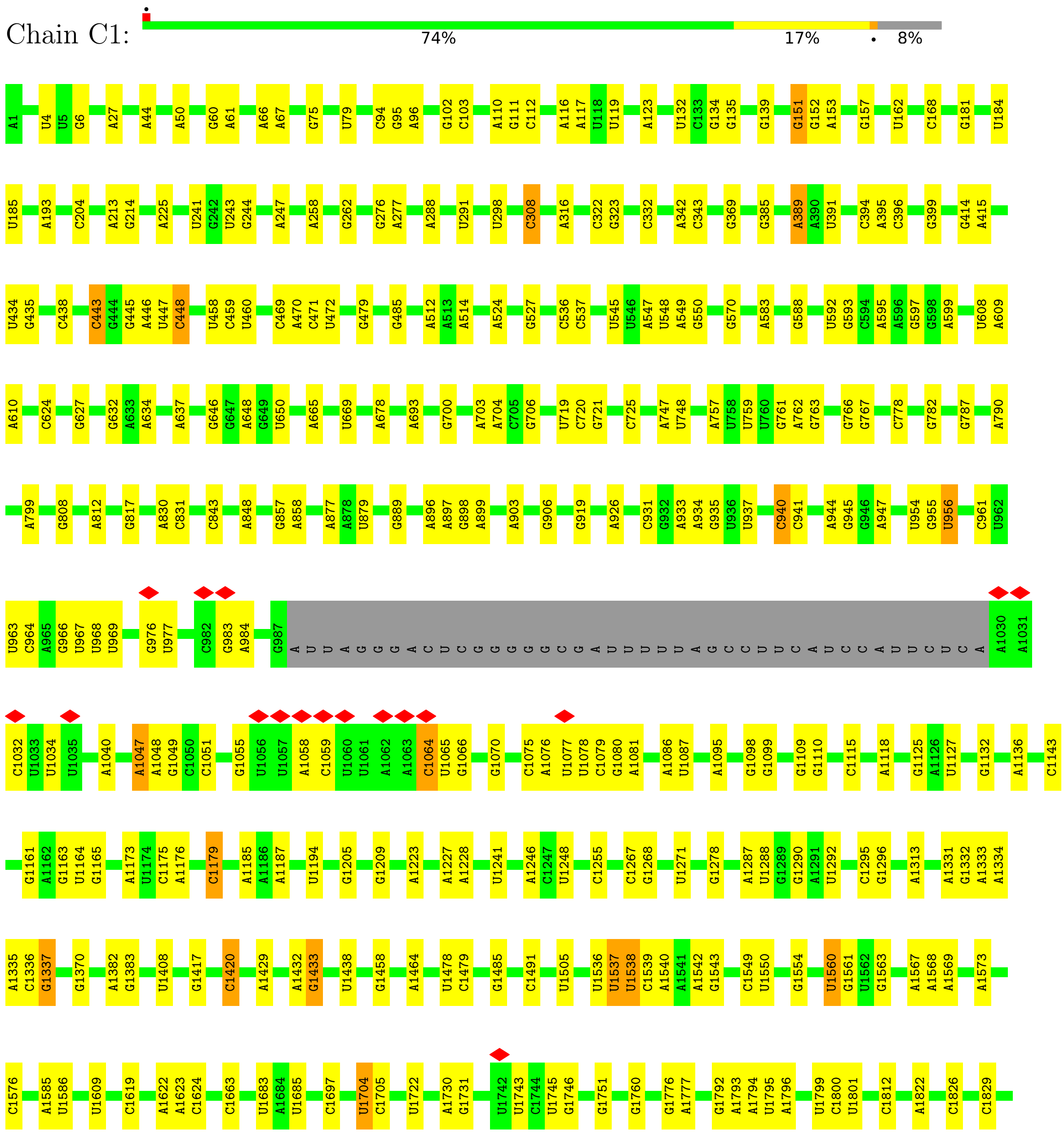
- Molecule 62 is water.

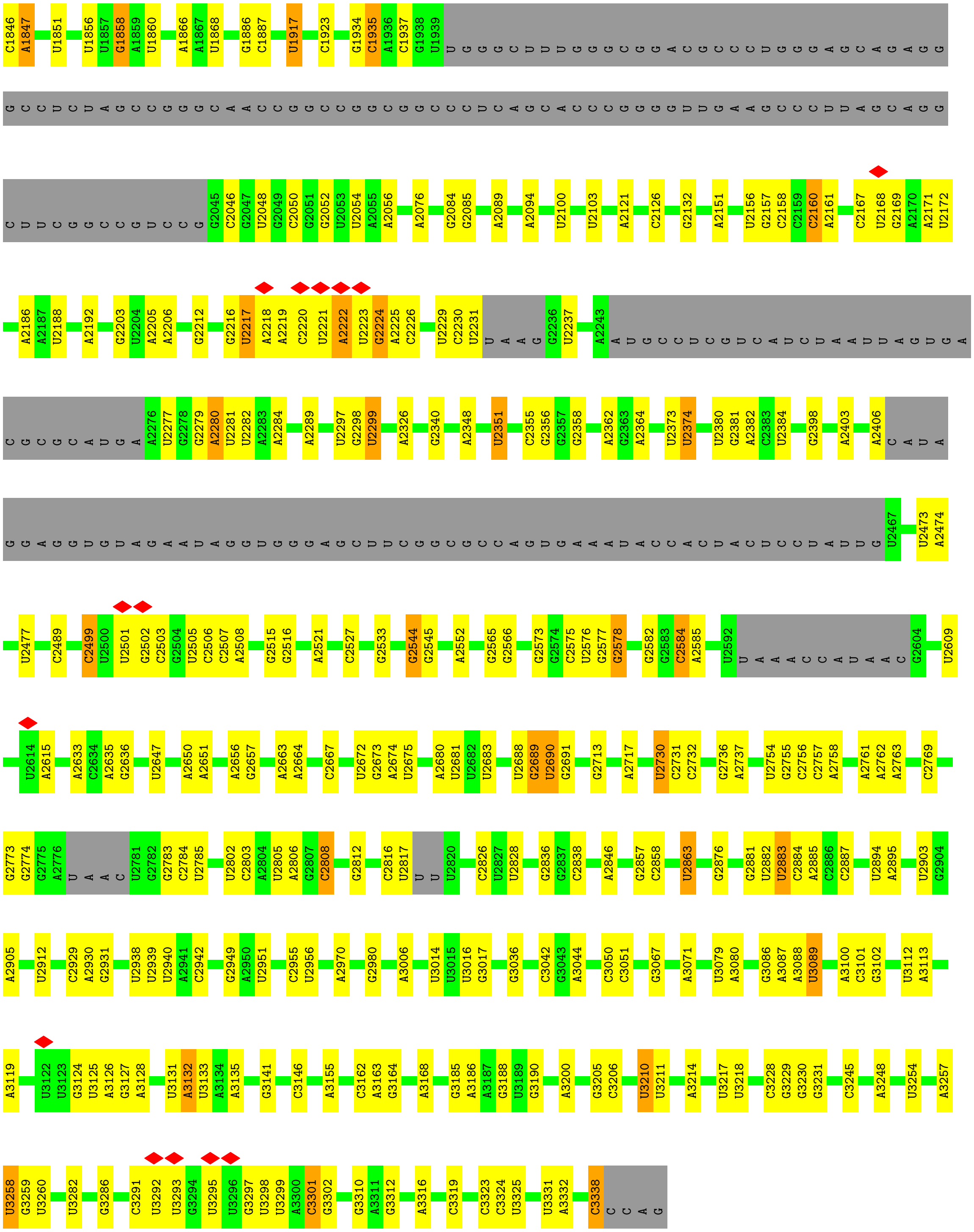
Mol	Chain	Residues	Atoms		AltConf
62	CH	1	Total 1	O 1	0
62	Cd	2	Total 2	O 2	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

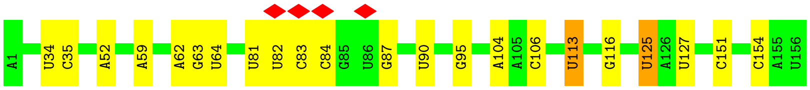
- Molecule 1: 26S rRNA





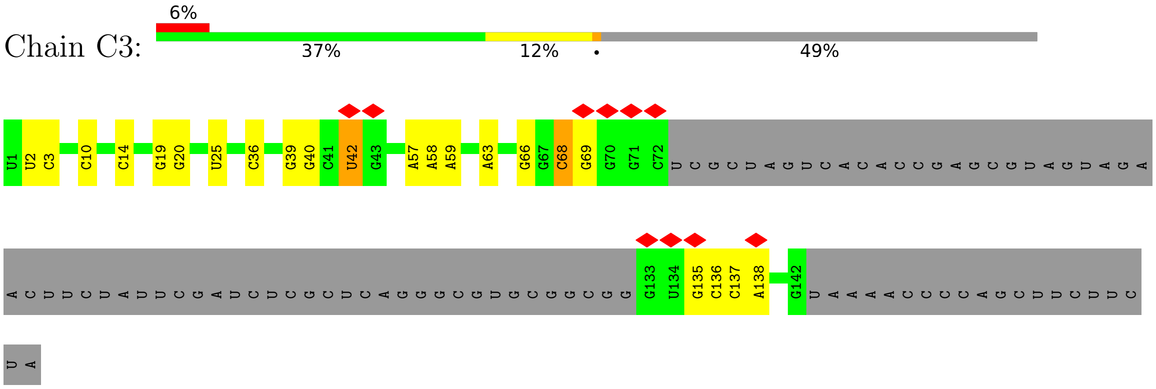
- Molecule 2: 5.8S rRNA

Chain C2:



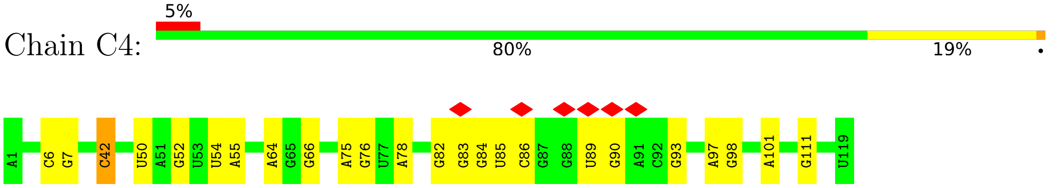
- Molecule 3: ITS2

Chain C3:



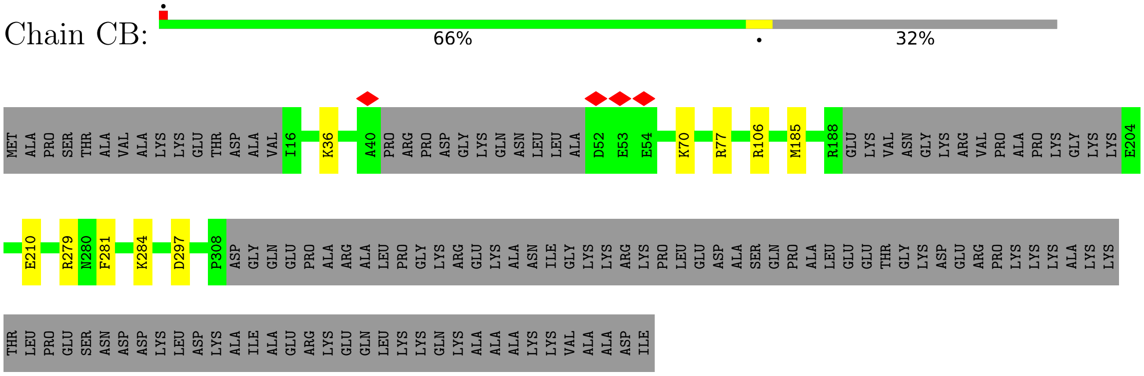
- Molecule 4: 5S rRNA

Chain C4:



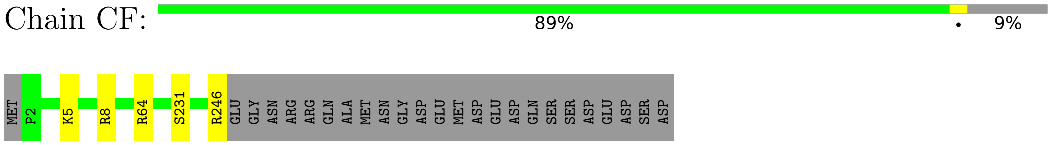
- Molecule 5: Utp30

Chain CB:



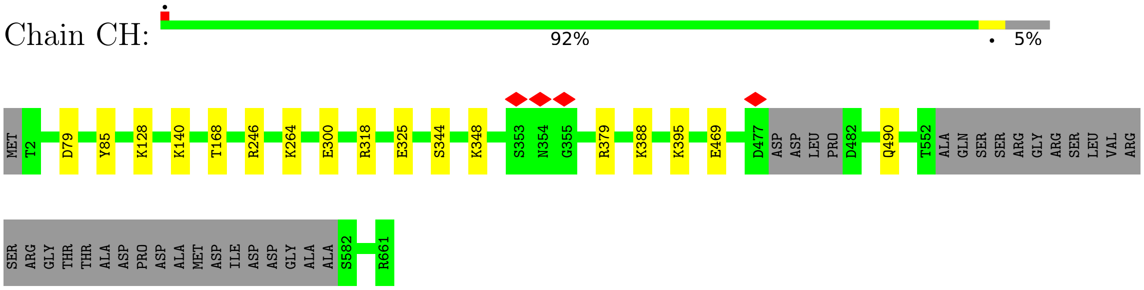
- Molecule 6: Large ribosomal subunit protein uL10

Chain CF:

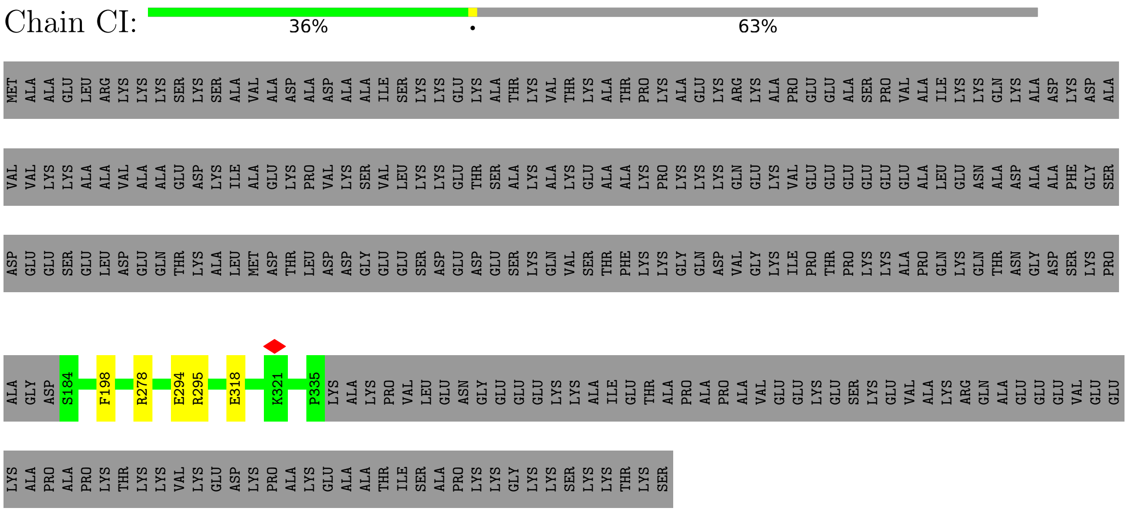


- Molecule 7: Nucleolar GTP-binding protein 1

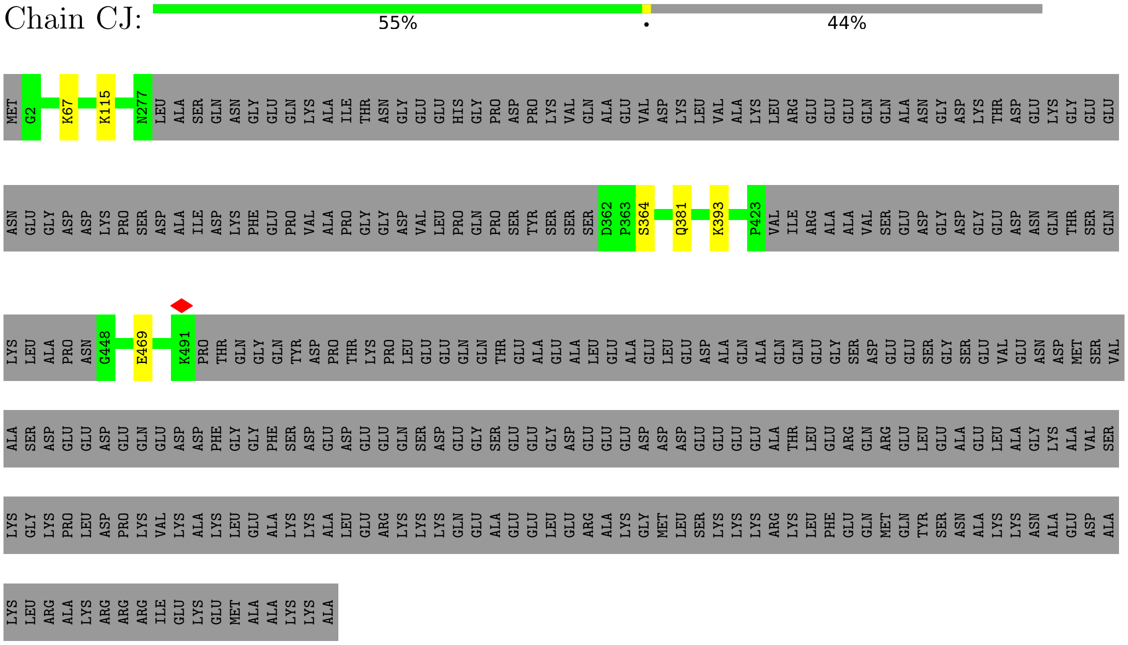
Chain CH:



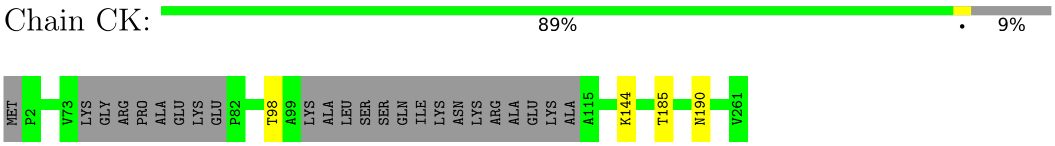
- Molecule 8: Putative RNA-binding protein



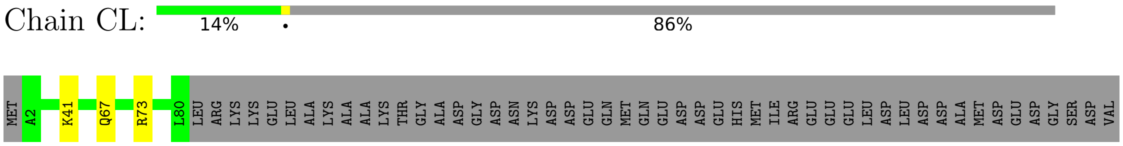
- Molecule 9: Pescadillo homolog

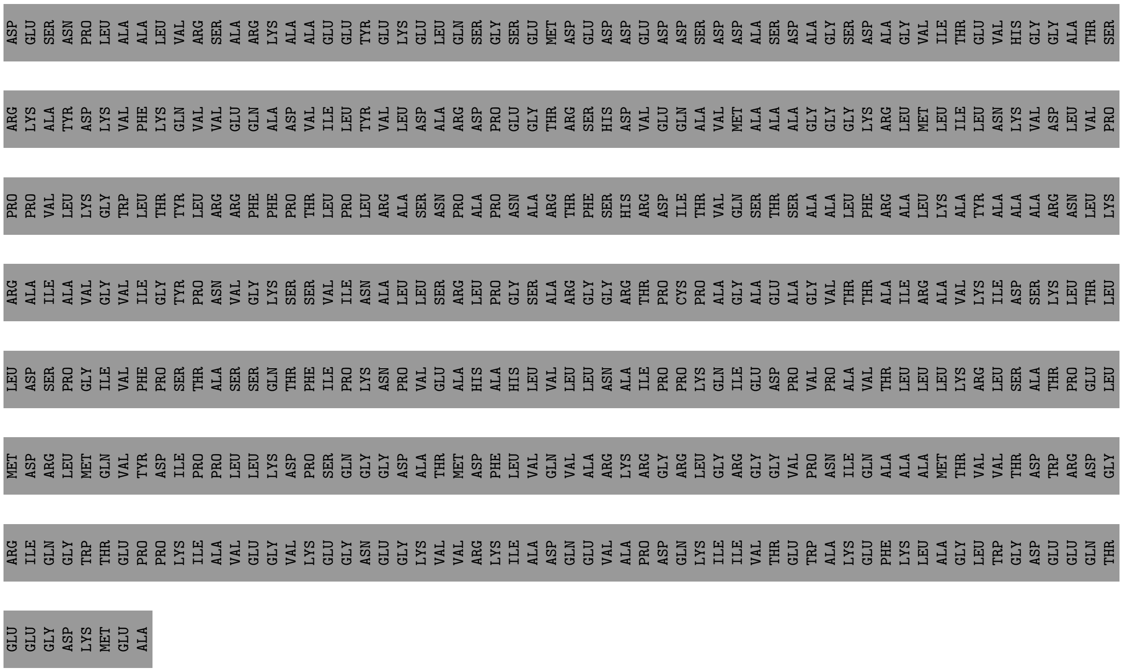


- Molecule 10: Ribosome biogenesis protein NSA2 homolog

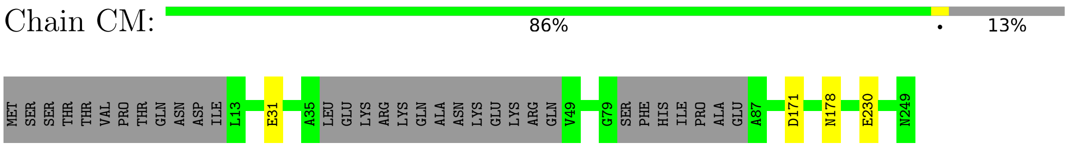


- Molecule 11: Putative GTP binding protein

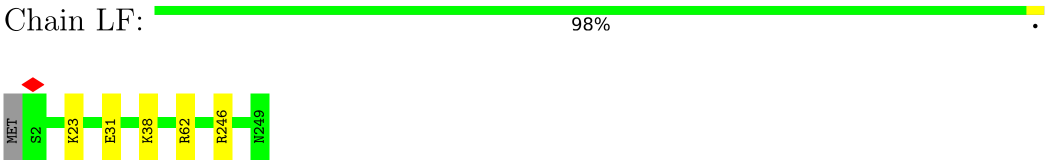




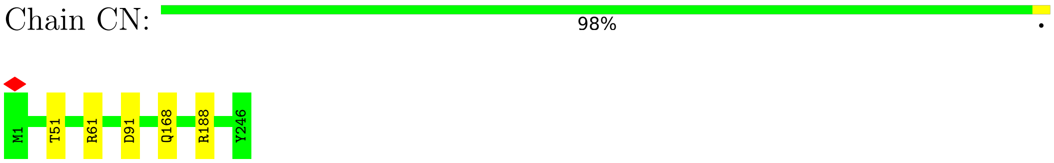
- Molecule 12: 60S ribosomal protein l7-like protein



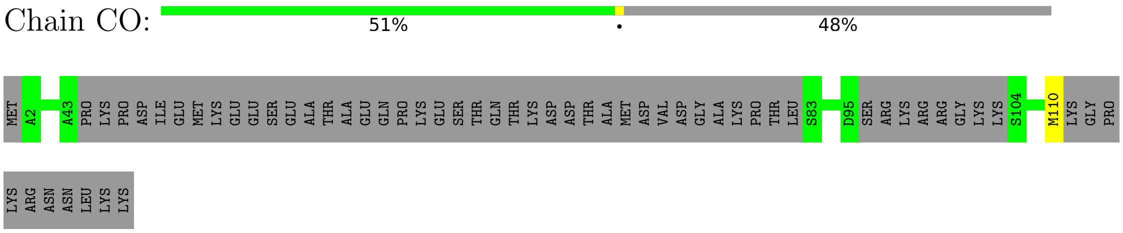
- Molecule 12: 60S ribosomal protein l7-like protein



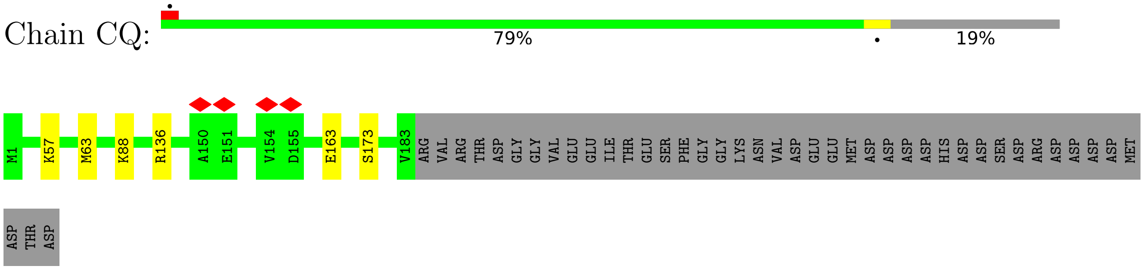
- Molecule 13: Eukaryotic translation initiation factor 6



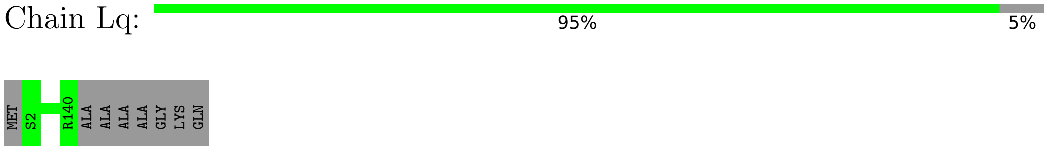
- Molecule 14: DUF2423 domain-containing protein



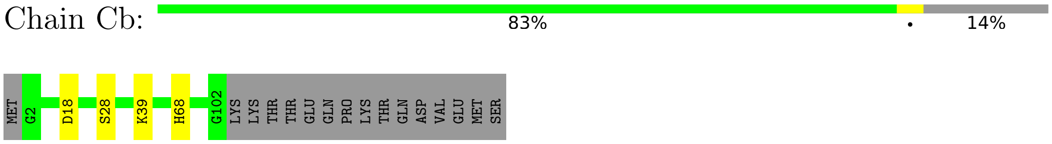
- Molecule 15: Ribosome biogenesis protein RLP24



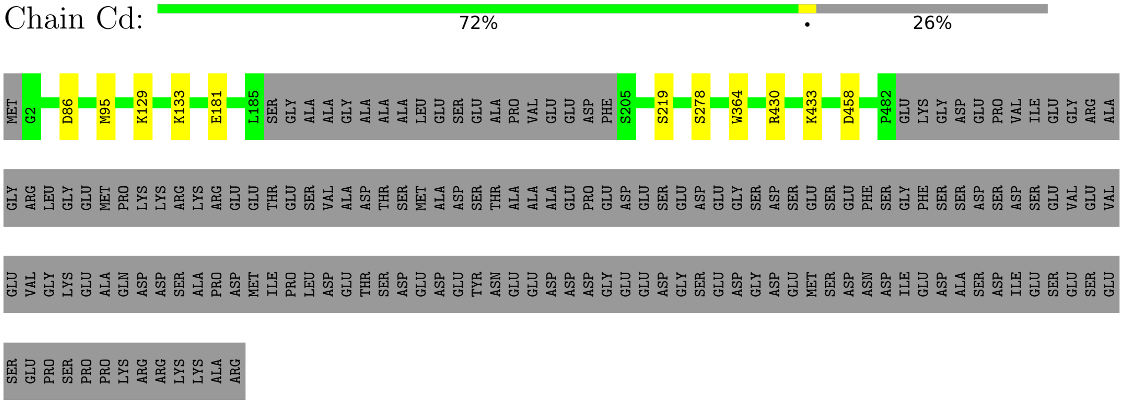
- Molecule 16: Putative 60S ribosomal protein



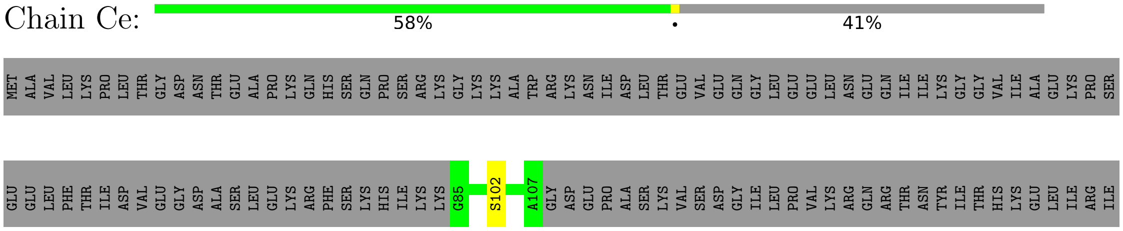
- Molecule 17: Zinc finger domain-containing protein

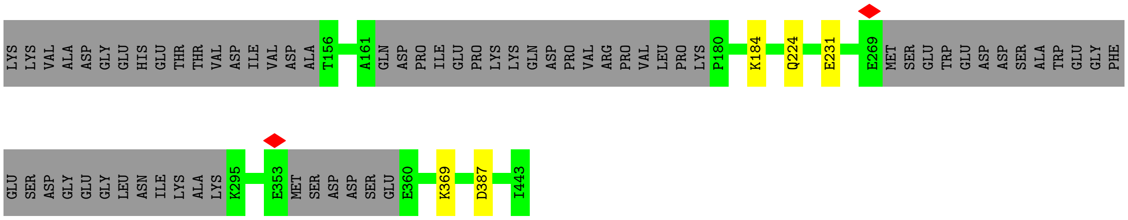


- Molecule 18: Nucleolar GTP-binding protein 2



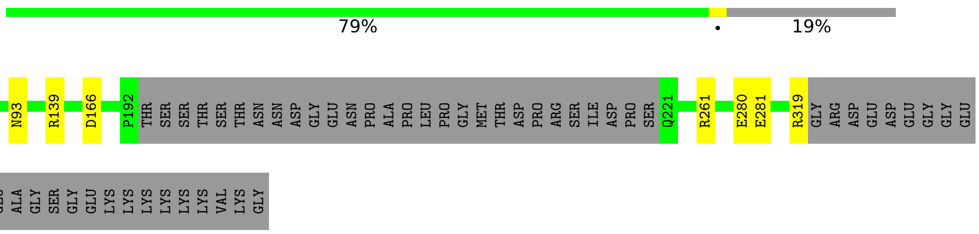
- Molecule 19: Ribosome biogenesis protein NOP53





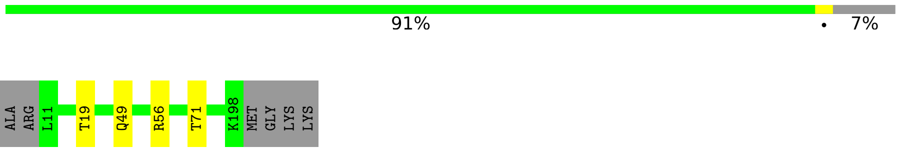
- Molecule 20: Ribosome production factor 2 homolog

Chain Cf:



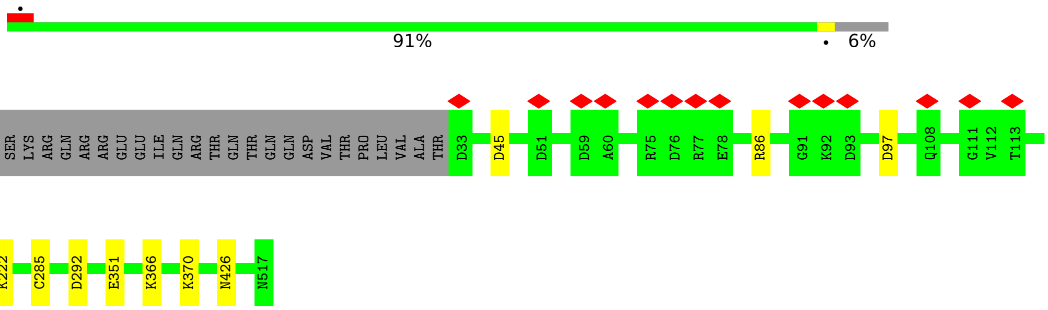
- Molecule 21: Ribosome biogenesis regulatory protein

Chain Cg:



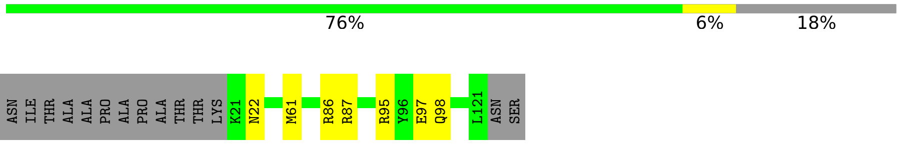
- Molecule 22: Ribosome assembly protein 4

Chain Ch:



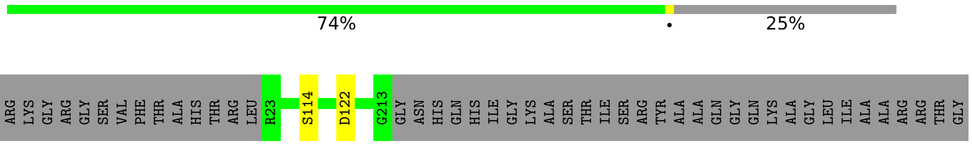
- Molecule 23: rRNA-processing protein

Chain Cz:

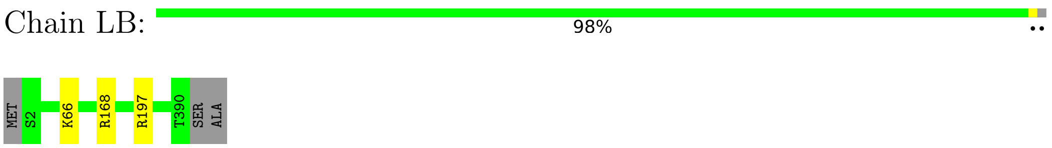


- Molecule 24: 60S ribosomal protein L2-like protein

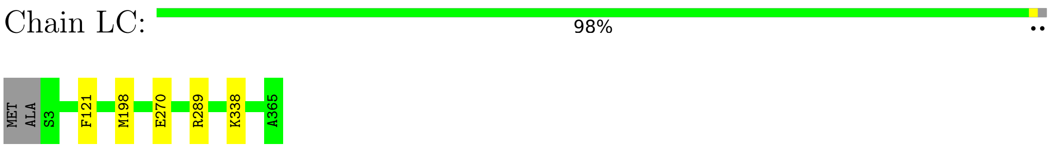
Chain LA:



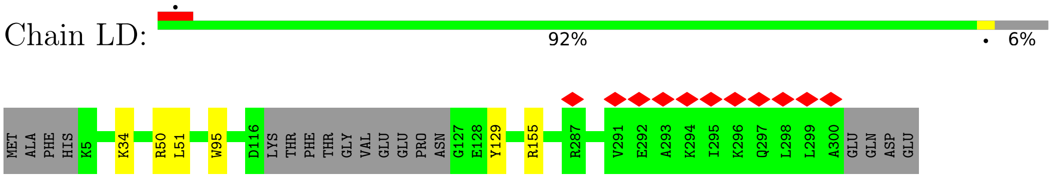
- Molecule 25: 60S ribosomal protein L3-like protein



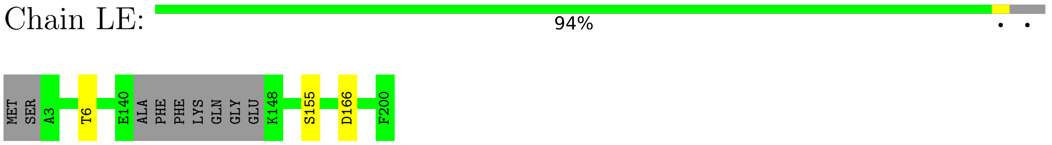
- Molecule 26: 60S ribosomal protein L4-like protein



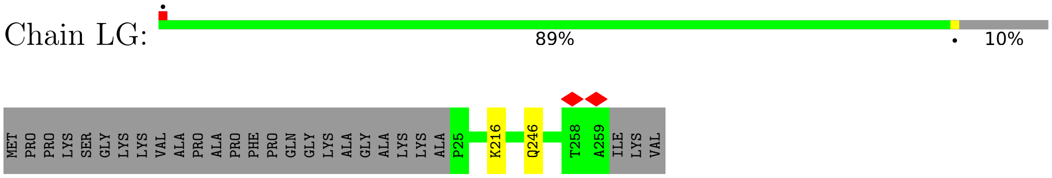
- Molecule 27: 60S ribosomal protein l5-like protein



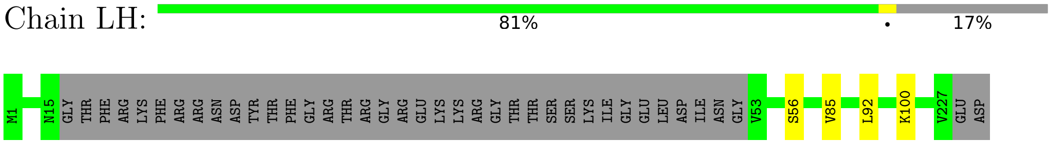
- Molecule 28: 60S ribosomal protein L6



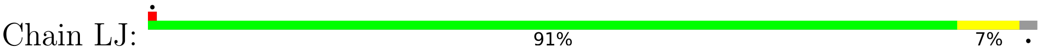
- Molecule 29: 60S ribosomal protein L8

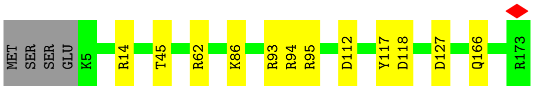


- Molecule 30: 60S ribosomal protein l9-like protein



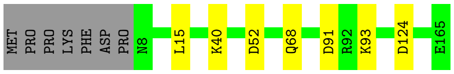
- Molecule 31: Putative ribosomal protein



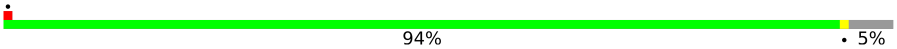


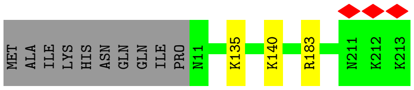
- Molecule 32: 60S ribosomal protein L12-like protein

Chain LK:

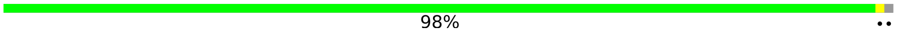



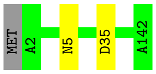
- Molecule 33: 60S ribosomal protein L13

Chain LL:




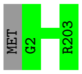
- Molecule 34: 60S ribosomal protein L14-like protein

Chain LM:


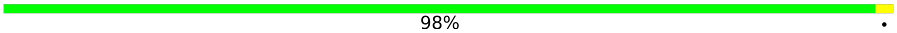


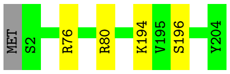
- Molecule 35: Ribosomal protein L15

Chain LN:

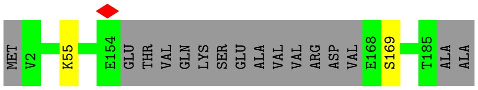
- Molecule 36: 60S ribosomal protein L16-like protein

Chain LO:




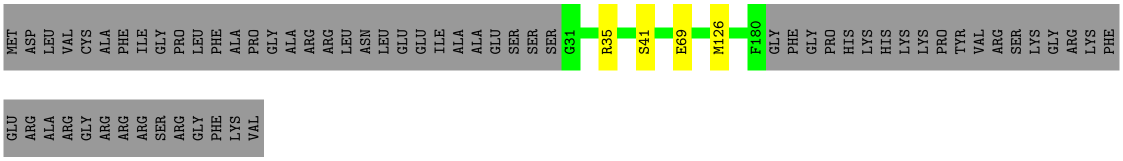
- Molecule 37: 60S ribosomal protein l17-like protein

Chain LP:

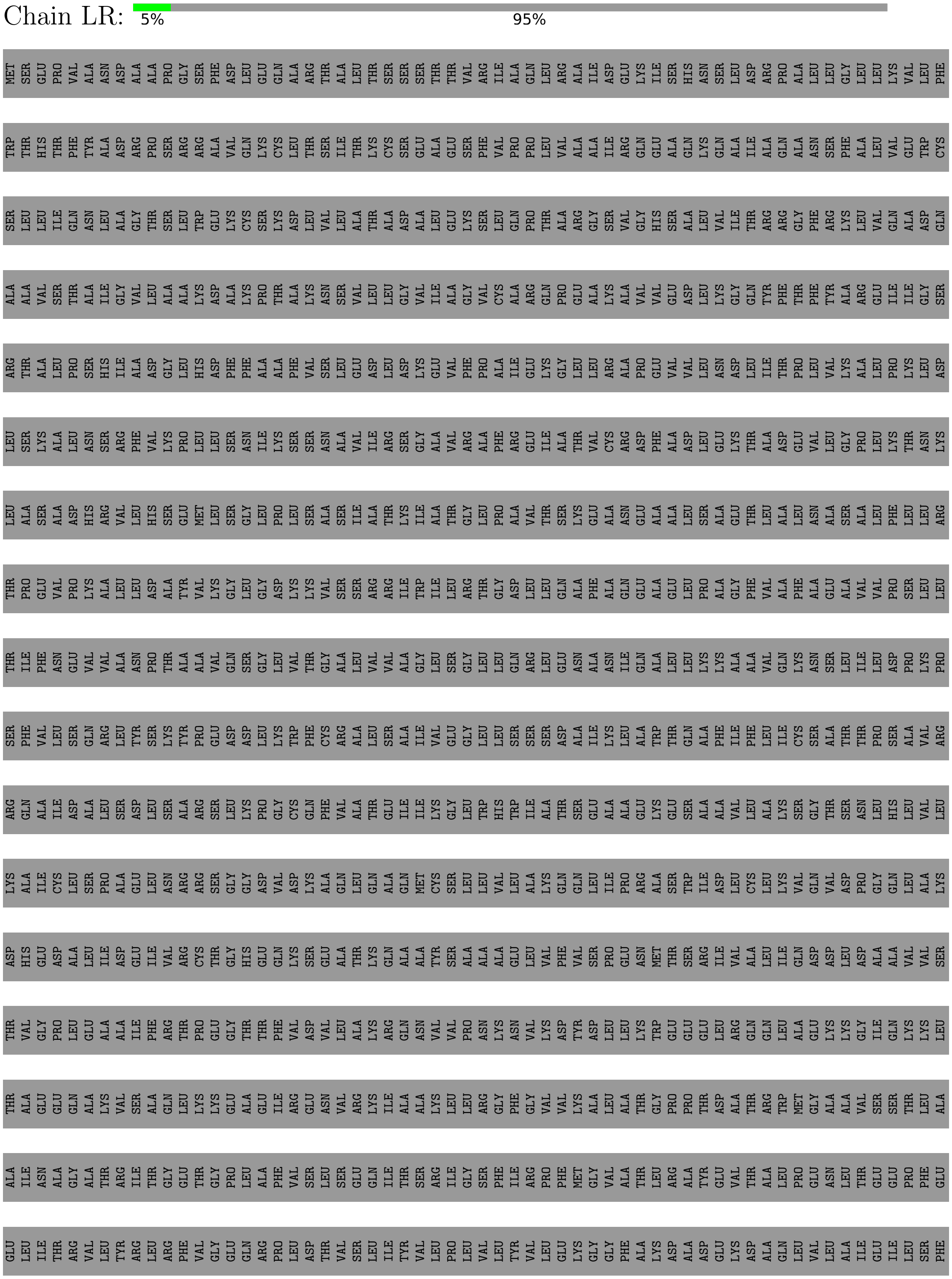



- Molecule 38: Ribosomal protein L18-like protein

Chain LQ:

- Molecule 39: Ribosomal protein L19



HIS THR ASP VAL ALA PHE ASP GLU ALA LEU PRO ARG ALA GLU ILE LEU SER SER LEU ILE SER SER MET GLN LYS TYR SER GLN HIS TYR LYS ILE LEU LYS ASP CYS PHE SER ASP MET VAL ARG CYS ILE ALA PRO ASN ILE SER PRO ALA GLU ILE GLY VAL LEU ALA ARG GLY ALA

ILE VAL PRO GLN THR SER VAL ARG THR ALA VAL LEU GLN ALA ILE SER ALA ASP VAL ASP MET SER ASP VAL ASN ALA SER GLU GLU ILE TRP LEU ALA CYS HIS ASP ASP ILE ASP GLU ASN ALA GLU LEU GLY ARG GLU ILE TRP GLU GLU SER GLU TRP LYS THR SER GLU GLU LEU

GLY HIS LYS MET ILE PRO TYR LEU GLU SER LYS ASP VAL GLN LEU ARG ARG ALA ALA ALA LYS SER LEU ALA GLU VAL ALA GLY GLN HIS PRO ASP VAL VAL ALA PRO ILE LEU GLU LYS LEU ARG GLU SER TYR VAL GLU LEU ALA LYS PRO ARG VAL GLN GLN LEU ASP GLU PHE GLY

MET PRO LYS LYS MET ASP LEU SER ASP PRO TRP GLU ALA ARG HIS GLY ILE ALA LEU ALA PHE LYS GLY LEU ALA PRO HIS LEU GLU LYS ARG GLN LEU GLU PRO TYR PHE ASN PHE LEU ILE GLU GLN GLY PRO LEU GLY ASP GLN SER ALA GLY VAL ARG ALA GLU MET LEU GLU ALA

ALA ASN MET THR ILE GLU ILE HIS GLY LYS GLU ILE LEU ASP ARG LEU MET LYS THR PHE GLU LYS VAL LEU GLU ALA PRO ASP LYS ASN SER GLU ALA ALA ASP ARG VAL ASN GLU ALA VAL ILE ILE MET TYR GLY ALA LEU ALA ARG HIS LEU LYS PRO GLY ASP LYS LYS ILE PRO

VAL VAL ILE GLU ARG LEU LEU ALA THR LEU SER THR PRO SER GLU ALA VAL GLN TYR ALA ILE ALA GLU CYS LEU PRO PRO LEU VAL ARG THR CYS ALA ASP LYS SER SER LYS TYR PHE ASP GLU MET MET GLU ILE LEU LEU THR SER LYS LYS TYR SER GLU GLN ARG GLY ALA ALA

TYR GLY LEU ALA GLY LEU VAL LEU GLY ARG GLY ILE ASN VAL LEU LYS GLU TYR ARG ILE MET THR GLN LEU ASN SER ALA LEU GLU ASN LYS LYS GLU ILE ARG GLN ARG GLU SER ALA MET ILE ALA TYR GLU LEU LEU SER THR ILE LEU GLY ARG LEU PHE GLU PRO TYR VAL ILE

GLN ILE VAL PRO GLN LEU LEU ALA GLY PHE GLY ASP GLY ASN ALA ASP VAL ARG GLU ALA ALA LEU ALA ALA LYS ALA CYS PHE ALA LYS LEU SER SER TYR GLY VAL LYS GLN ILE LEU PRO THR LEU LEU ASN GLY LEU ASP ASP ASP GLN TRP ARG SER LYS LYS GLY ALA CYS

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LEU MET GLN THR LEU LYS SER ASP THR SER ALA GLY ASP ARG LEU GLY SER ALA GLN ALA LEU SER GLU VAL LEU ALA GLY LEU GLY THR SER ARG LEU GLU GLU THR LEU PRO THR ILE LEU GLN ASN VAL GLU SER PRO LYS PRO ALA VAL ARG GLU GLY PHE MET SER LEU PHE ILE

PHE LEU PRO VAL CYS PHE GLY ASN SER PHE ALA ASN TYR LEU GLY LYS ILE ILE PRO PRO ILE LEU SER GLY LEU ALA ASP ASP VAL GLU SER ILE ARG GLU THR ALA LEU ARG ALA GLY ARG LEU LEU VAL LYS ASN PHE ALA VAL ARG ALA VAL ASP LEU LEU LEU PRO GLU LEU GLU

ARG GLY LEU ALA ASP ASP ASN TYR ARG ILE ARG LEU SER SER VAL GLU LEU VAL GLY ASP LEU LEU PHE ASN LEU ALA GLY VAL LYS ALA SER ALA ASN LYS GLU GLU ASP GLU ALA ASP GLN ASP ILE THR LYS GLU ALA GLY ALA SER LEU ARG GLU VAL LEU GLY GLU GLU LYS ARG

ASN LYS ILE LEU SER ALA LEU TYR VAL CYS ARG CYS ASP THR ALA GLY ALA VAL ARG ALA ALA ALA VAL THR VAL TRP LYS GLN LEU VAL HIS SER PRO ARG THR LEU LYS GLU LEU VAL PRO THR LEU THR GLN LEU LEU ILE LYS ARG LEU GLY SER SER ASN MET GLU HIS LYS VAL

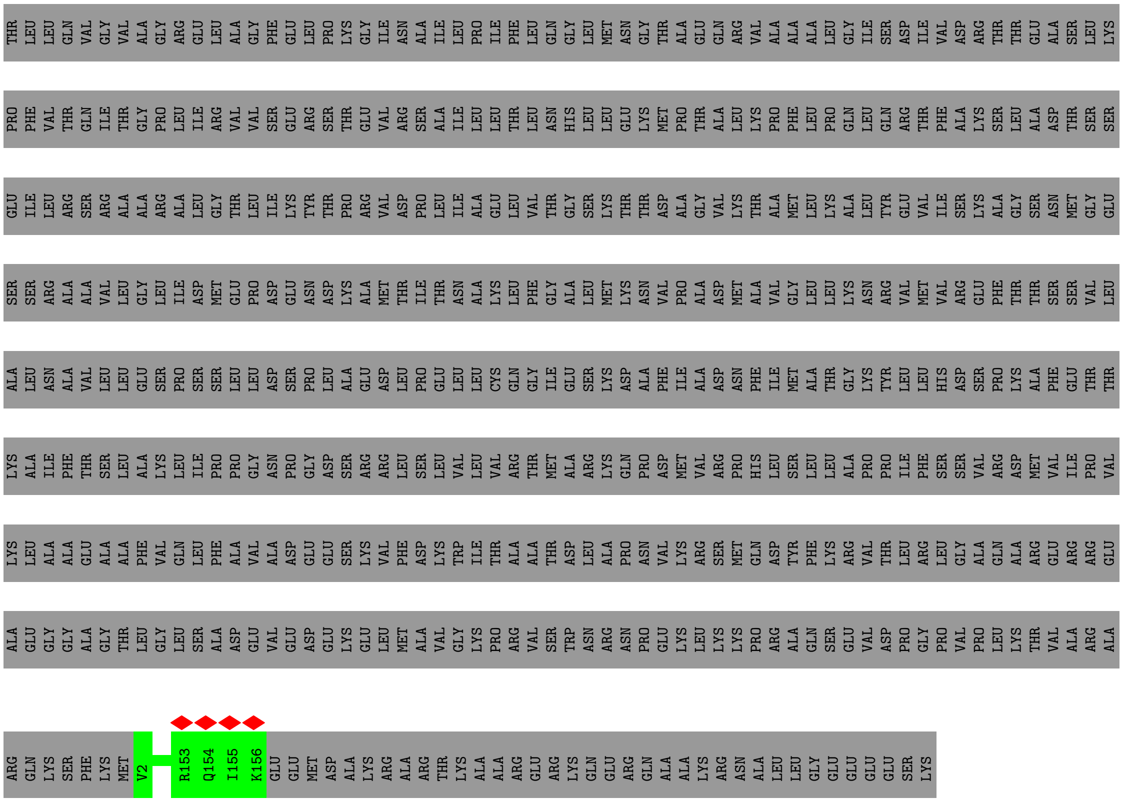
ILE ALA SER ASN ALA LEU GLY GLU LEU ILE LYS LYS ALA GLY ASP GLY VAL LEU ALA THR LEU LEU PRO THR LEU GLU GLU GLY LEU GLN THR SER ARG ASP VAL ASN ALA LYS GLN GLY ILE CYS LEU ALA LEU LYS GLU LEU ILE SER SER ALA SER PRO GLU ALA LEU GLU ASP HIS

GLU LYS THR LEU ILE SER VAL VAL ARG THR ALA LEU THR ASP SER ASP SER ASP VAL ARG GLU ALA ALA ALA GLU ALA PHE ASP SER LEU GLN GLN ILE ILE GLY LYS ARG ALA ILE ASP GLN VAL LEU PRO PHE LEU LEU ASN LEU LEU ARG SER GLU GLU GLU ALA ASN ASN ALA LEU

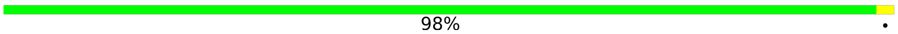
ALA ALA LEU LEU THR LEU LEU THR GLU PRO THR ARG ALA ASN ILE ILE LEU PRO ASN LEU ILE PRO THR LEU ILE THR PRO PRO ILE SER ALA PHE ASN ALA LYS ALA LEU ALA SER LEU SER LYS VAL ALA GLY ALA ALA MET ASN ARG ARG LEU PRO ASN ILE ILE ASN SER LEU MET

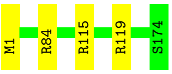
ASP ASN ILE VAL GLY CYS ALA ASP GLU THR LEU ARG GLU GLU LEU ASP THR SER PHE ASP THR VAL ILE LEU SER ILE ASP ASP THR ASP GLY LEU ASN VAL VAL MET ASN VAL LEU LEU GLN LEU ILE LYS HIS GLU ASP HIS ARG LYS ARG ALA ALA THR GLY ARG HIS LEU ALA LYS

PHE PHE SER ALA ALA THR VAL ASN TYR SER ARG TYR ASN GLN ASP ILE ILE ARG ALA LEU LEU ILE SER PHE ASP ASP LYS ASP MET GLU VAL VAL LYS ALA SER TRP ASN ALA LEU ASN GLU PHE THR LYS ARG LEU LYS LYS GLU GLU MET GLU GLY LEU VAL ILE SER THR ARG GLN



- Molecule 40: 60S ribosomal protein L20

Chain LS:


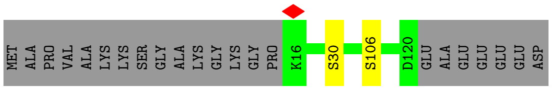


- Molecule 41: 60S ribosomal protein l21-like protein

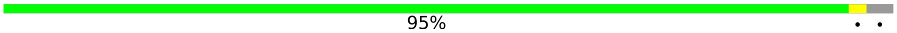
Chain LT:

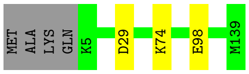

- Molecule 42: 60S ribosomal protein L22-like protein

Chain LU:

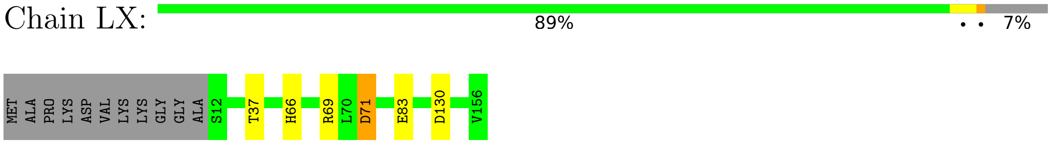



- Molecule 43: 60S ribosomal protein l23-like protein

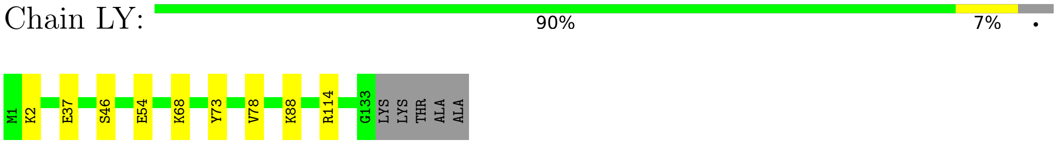
Chain LV:




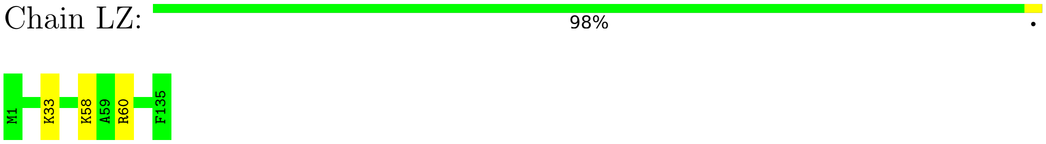
- Molecule 44: 60S ribosomal protein L25-like protein



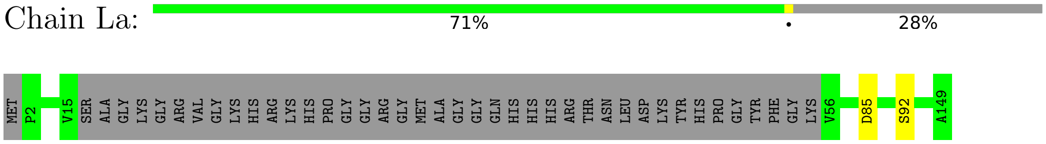
- Molecule 45: 60S ribosomal protein L26-like protein



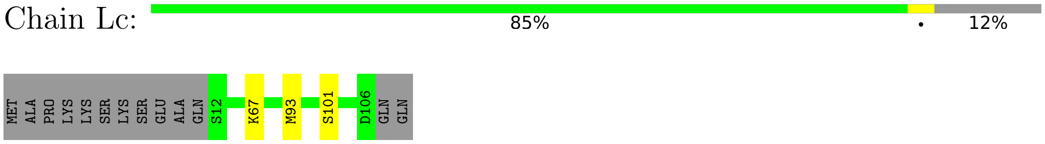
- Molecule 46: 60S ribosomal protein L27



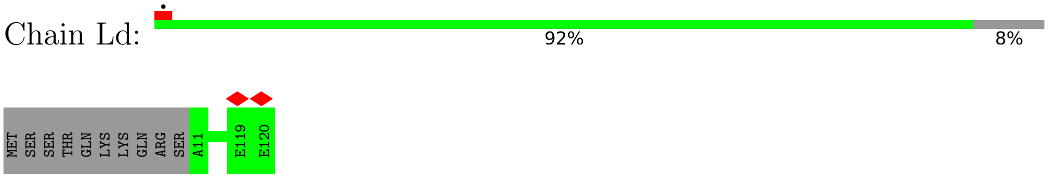
- Molecule 47: 60S ribosomal protein L28-like protein



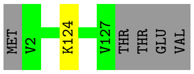
- Molecule 48: 60S ribosomal protein l30-like protein



- Molecule 49: Putative 60S ribosomal protein

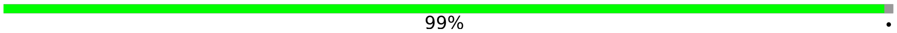


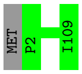
- Molecule 50: 60S ribosomal protein L32-like protein



- Molecule 51: 60S ribosomal protein l33-like protein

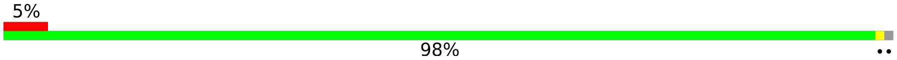
Chain Lf:

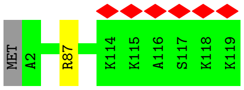




- Molecule 52: Ribosomal protein l34-like protein

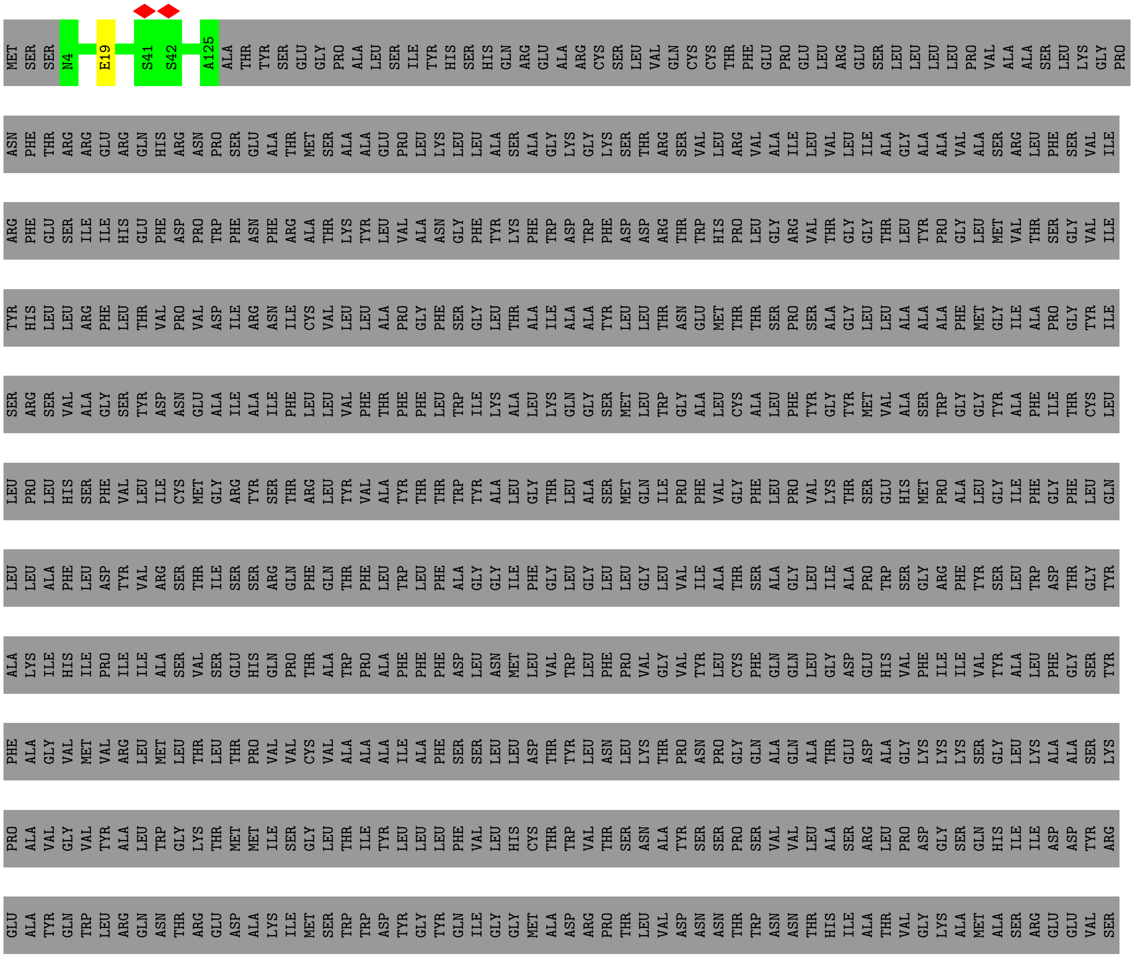
Chain Lg:

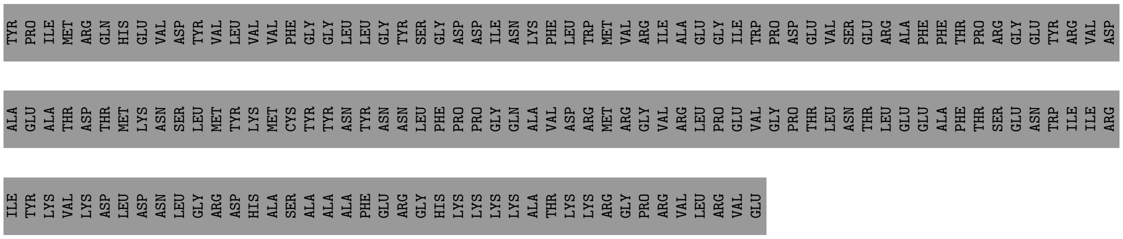




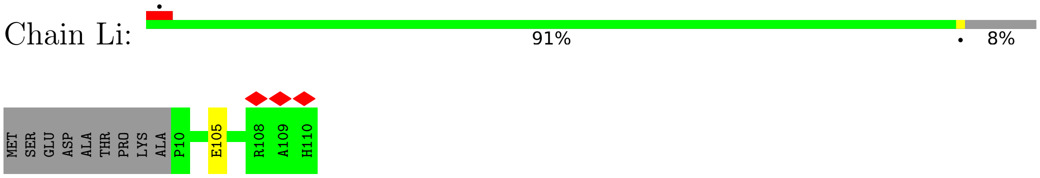
- Molecule 53: dolichyl-diphosphooligosaccharide--protein glycotransferase

Chain Lh:

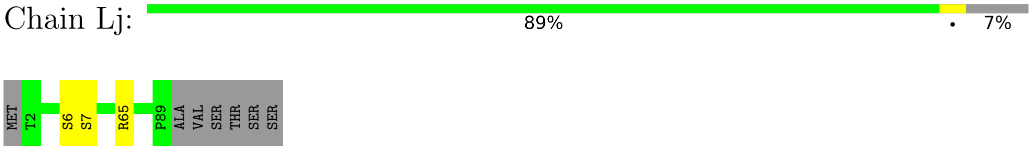




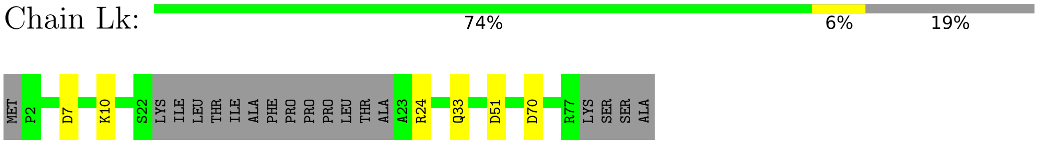
- Molecule 54: 60S ribosomal protein L36



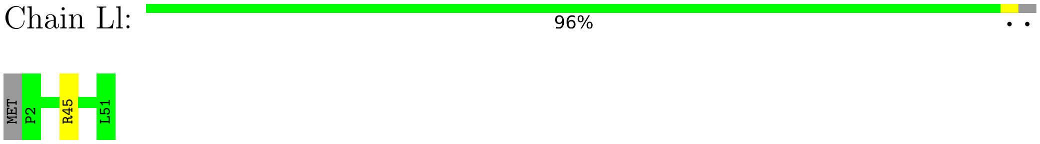
- Molecule 55: Ribosomal protein L37



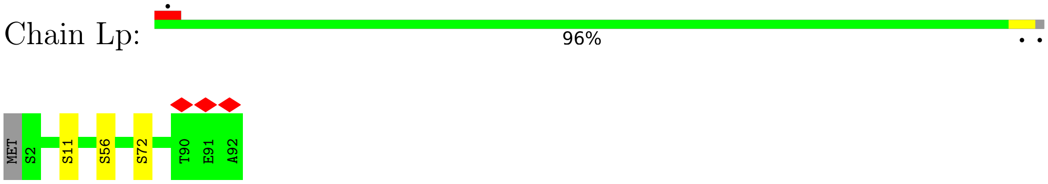
- Molecule 56: 60S ribosomal protein L38-like protein



- Molecule 57: Ribosomal protein eL39



- Molecule 58: 60S ribosomal protein L43-like protein



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	745895	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	45.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	10.768	Depositor
Minimum map value	0.000	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.175	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	522.5, 522.5, 522.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, OMG, ZN, OMU, A2M, MG, OMC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	C1	0.55	0/72882	0.95	123/113631 (0.1%)
2	C2	0.55	0/3710	0.90	5/5778 (0.1%)
3	C3	0.44	0/1958	0.98	4/3050 (0.1%)
4	C4	0.45	0/2833	0.98	3/4414 (0.1%)
5	CB	0.29	0/2166	0.52	0/2945
6	CF	0.32	0/1972	0.57	0/2660
7	CH	0.30	0/5147	0.56	0/6926
8	CI	0.37	0/1265	0.67	1/1702 (0.1%)
9	CJ	0.32	0/3196	0.53	0/4319
10	CK	0.31	0/1939	0.57	0/2608
11	CL	0.29	0/631	0.59	0/843
12	CM	0.34	0/1805	0.60	1/2417 (0.0%)
12	LF	0.34	0/2061	0.55	0/2765
13	CN	0.28	0/1878	0.56	0/2555
14	CO	0.31	0/470	0.53	0/619
15	CQ	0.32	0/1504	0.60	0/2000
16	Lq	0.30	0/1091	0.58	0/1468
17	Cb	0.29	0/845	0.59	0/1128
18	Cd	0.30	0/3770	0.54	1/5082 (0.0%)
19	Ce	0.30	0/2173	0.57	0/2890
20	Cf	0.29	0/2326	0.56	0/3113
21	Cg	0.31	0/1508	0.57	0/2051
22	Ch	0.30	0/3914	0.60	0/5319
23	Cz	0.33	0/877	0.65	1/1148 (0.1%)
24	LA	0.33	0/1488	0.61	1/2009 (0.0%)
25	LB	0.30	0/3172	0.56	0/4260
26	LC	0.30	0/2808	0.53	0/3785
27	LD	0.31	0/2308	0.54	0/3105
28	LE	0.30	0/1504	0.56	1/2027 (0.0%)
29	LG	0.34	0/1918	0.54	0/2565
30	LH	0.34	0/1515	0.58	1/2037 (0.0%)
31	LJ	0.30	0/1379	0.65	1/1844 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	LK	0.30	0/1198	0.61	2/1611 (0.1%)
33	LL	0.28	0/1614	0.57	0/2168
34	LM	0.31	0/1145	0.57	0/1539
35	LN	0.33	0/1741	0.62	0/2332
36	LO	0.33	0/1645	0.55	0/2205
37	LP	0.29	0/1364	0.58	0/1835
38	LQ	0.31	0/1218	0.59	0/1639
39	LR	0.29	0/1260	0.56	0/1683
40	LS	0.32	0/1461	0.58	0/1966
41	LT	0.33	0/1046	0.59	0/1409
42	LU	0.30	0/859	0.54	0/1151
43	LV	0.30	0/1009	0.57	1/1357 (0.1%)
44	LX	0.31	0/1151	0.59	2/1547 (0.1%)
45	LY	0.30	0/1070	0.61	0/1432
46	LZ	0.32	0/1135	0.60	0/1519
47	La	0.30	0/892	0.54	0/1200
48	Lc	0.30	0/714	0.49	0/960
49	Ld	0.28	0/889	0.55	0/1192
50	Le	0.29	0/1035	0.57	0/1379
51	Lf	0.31	0/883	0.56	0/1187
52	Lg	0.30	0/927	0.60	0/1244
53	Lh	0.31	0/1014	0.56	0/1349
54	Li	0.31	0/834	0.65	0/1099
55	Lj	0.30	0/712	0.63	0/944
56	Lk	0.29	0/640	0.53	0/850
57	Ll	0.27	0/446	0.57	0/593
58	Lp	0.31	0/706	0.67	0/940
All	All	0.44	0/166621	0.79	148/241393 (0.1%)

There are no bond length outliers.

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	1538	U	N3-C2-O2	-10.53	114.83	122.20
1	C1	1179	C	C2-N1-C1'	10.46	130.31	118.80
1	C1	1538	U	N1-C2-O2	10.06	129.84	122.80
1	C1	1179	C	N1-C2-O2	9.60	124.66	118.90
1	C1	1538	U	C2-N1-C1'	9.24	128.79	117.70
1	C1	399	G	O4'-C1'-N9	8.83	115.26	108.20
1	C1	1935	C	C2-N1-C1'	8.43	128.07	118.80
1	C1	2730	U	N1-C2-O2	8.28	128.60	122.80
1	C1	2730	U	C2-N1-C1'	8.26	127.61	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	1478	U	C2-N1-C1'	8.10	127.42	117.70
12	CM	171	ASP	CB-CG-OD2	7.88	125.39	118.30
1	C1	2730	U	N3-C2-O2	-7.86	116.70	122.20
1	C1	2351	U	N3-C2-O2	-7.75	116.77	122.20
1	C1	2681	U	N3-C2-O2	-7.63	116.86	122.20
1	C1	1179	C	C6-N1-C1'	-7.58	111.71	120.80
1	C1	1478	U	N1-C2-O2	7.33	127.93	122.80
1	C1	1179	C	N3-C2-O2	-7.24	116.83	121.90
1	C1	1478	U	N3-C2-O2	-7.22	117.14	122.20
31	LJ	118	ASP	CB-CG-OD1	7.18	124.76	118.30
1	C1	3089	U	C2-N1-C1'	7.16	126.28	117.70
1	C1	2544	G	N3-C4-N9	7.12	130.27	126.00
1	C1	961	C	C2-N1-C1'	7.00	126.50	118.80
24	LA	122	ASP	CB-CG-OD1	6.98	124.58	118.30
1	C1	2689	G	C4-N9-C1'	6.86	135.42	126.50
1	C1	2374	U	N3-C2-O2	-6.82	117.43	122.20
1	C1	79	U	N3-C2-O2	-6.64	117.55	122.20
1	C1	1479	C	C2-N1-C1'	6.54	125.99	118.80
1	C1	103	C	N1-C2-O2	6.50	122.80	118.90
32	LK	124	ASP	CB-CG-OD2	6.50	124.14	118.30
2	C2	125	U	N1-C2-O2	6.48	127.34	122.80
1	C1	940	C	C2-N1-C1'	6.47	125.92	118.80
1	C1	1064	C	P-O3'-C3'	6.44	127.43	119.70
2	C2	125	U	C2-N1-C1'	6.44	125.43	117.70
1	C1	103	C	N3-C2-O2	-6.39	117.43	121.90
1	C1	961	C	N3-C2-O2	-6.38	117.43	121.90
44	LX	71	ASP	CB-CG-OD1	6.38	124.04	118.30
1	C1	2544	G	N3-C4-C5	-6.36	125.42	128.60
1	C1	817	G	O4'-C1'-N9	6.28	113.23	108.20
1	C1	151	G	P-O3'-C3'	6.20	127.14	119.70
3	C3	14	C	C2-N1-C1'	6.20	125.62	118.80
1	C1	2689	G	N3-C4-N9	6.18	129.71	126.00
1	C1	2544	G	C4-N9-C1'	6.18	134.53	126.50
1	C1	3016	U	C2-N1-C1'	6.14	125.06	117.70
43	LV	29	ASP	CB-CG-OD1	6.10	123.79	118.30
2	C2	64	U	N3-C2-O2	-6.09	117.93	122.20
1	C1	1704	U	O4'-C1'-N1	6.08	113.07	108.20
1	C1	1337	G	C4-N9-C1'	6.07	134.39	126.50
1	C1	1537	U	P-O3'-C3'	6.07	126.98	119.70
1	C1	3258	U	P-O3'-C3'	6.07	126.98	119.70
2	C2	125	U	N3-C2-O2	-6.05	117.97	122.20
1	C1	2689	G	N3-C4-C5	-6.04	125.58	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	1408	U	N3-C2-O2	-6.04	117.97	122.20
1	C1	2681	U	N1-C2-O2	6.02	127.02	122.80
1	C1	2160	C	P-O3'-C3'	6.02	126.92	119.70
1	C1	1851	U	N3-C2-O2	-6.01	117.99	122.20
1	C1	1935	C	C6-N1-C1'	-5.95	113.66	120.80
1	C1	2217	U	C2-N1-C1'	5.95	124.84	117.70
1	C1	961	C	N1-C2-O2	5.93	122.46	118.90
1	C1	2689	G	C8-N9-C1'	-5.92	119.31	127.00
18	Cd	95	MET	CB-CG-SD	5.87	130.02	112.40
1	C1	3338	C	C2-N1-C1'	5.83	125.22	118.80
1	C1	1179	C	C6-N1-C2	-5.80	117.98	120.30
1	C1	2883	U	P-O3'-C3'	5.80	126.66	119.70
1	C1	961	C	C6-N1-C2	-5.79	117.98	120.30
1	C1	2299	U	N3-C2-O2	-5.77	118.16	122.20
1	C1	1560	U	N1-C2-O2	5.76	126.83	122.80
1	C1	2217	U	N1-C2-O2	5.76	126.83	122.80
32	LK	52	ASP	CB-CG-OD1	5.76	123.48	118.30
1	C1	1087	U	C2-N1-C1'	5.75	124.60	117.70
1	C1	3338	C	N1-C2-O2	5.74	122.34	118.90
1	C1	1479	C	C6-N1-C2	-5.73	118.01	120.30
4	C4	42	C	N1-C2-O2	5.71	122.33	118.90
1	C1	956	U	C2-N1-C1'	5.71	124.55	117.70
44	LX	130	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C1	1538	U	C6-N1-C2	-5.69	117.59	121.00
1	C1	1560	U	C2-N1-C1'	5.65	124.47	117.70
1	C1	1227	A	O4'-C1'-N9	5.62	112.69	108.20
1	C1	1087	U	N1-C2-O2	5.61	126.73	122.80
8	CI	294	GLU	C-N-CA	-5.60	107.70	121.70
1	C1	448	C	N1-C2-O2	5.59	122.26	118.90
1	C1	2505	U	C2-N1-C1'	5.59	124.41	117.70
1	C1	1560	U	N3-C2-O2	-5.59	118.29	122.20
1	C1	2351	U	N1-C2-O2	5.58	126.71	122.80
1	C1	1408	U	N1-C2-O2	5.57	126.70	122.80
1	C1	2217	U	N3-C2-O2	-5.57	118.30	122.20
1	C1	2374	U	N1-C2-O2	5.55	126.69	122.80
28	LE	166	ASP	CB-CG-OD2	5.54	123.29	118.30
1	C1	443	C	C2-N1-C1'	5.54	124.89	118.80
1	C1	3006	A	O4'-C1'-N9	5.54	112.63	108.20
1	C1	162	U	N3-C2-O2	-5.53	118.33	122.20
1	C1	1095	A	O4'-C1'-N9	5.51	112.61	108.20
1	C1	2808	C	C2-N1-C1'	5.50	124.85	118.80
1	C1	1337	G	C8-N9-C1'	-5.49	119.87	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	1478	U	C6-N1-C1'	-5.47	113.54	121.20
1	C1	1538	U	C6-N1-C1'	-5.47	113.54	121.20
1	C1	2224	G	C4-N9-C1'	5.47	133.61	126.50
1	C1	2863	U	C2-N1-C1'	5.46	124.25	117.70
1	C1	967	U	N3-C2-O2	-5.40	118.42	122.20
4	C4	50	U	N1-C2-O2	5.40	126.58	122.80
1	C1	897	A	C2-N3-C4	5.40	113.30	110.60
1	C1	1179	C	C5-C6-N1	5.39	123.70	121.00
1	C1	940	C	N1-C2-O2	5.39	122.14	118.90
1	C1	1271	U	N3-C2-O2	-5.39	118.43	122.20
3	C3	42	U	N1-C2-O2	5.38	126.57	122.80
1	C1	3301	C	P-O3'-C3'	5.37	126.14	119.70
1	C1	2499	C	C2-N1-C1'	5.36	124.70	118.80
1	C1	2280	A	P-O3'-C3'	5.36	126.13	119.70
1	C1	706	G	O4'-C1'-N9	5.35	112.48	108.20
1	C1	308	C	C2-N1-C1'	5.35	124.68	118.80
1	C1	2544	G	C2-N3-C4	5.34	114.57	111.90
1	C1	102	G	C8-N9-C1'	-5.34	120.05	127.00
1	C1	1935	C	C6-N1-C2	-5.34	118.17	120.30
1	C1	1047	A	P-O3'-C3'	5.33	126.09	119.70
1	C1	103	C	C6-N1-C2	-5.31	118.18	120.30
1	C1	1295	C	C6-N1-C2	-5.30	118.18	120.30
1	C1	3210	U	P-O3'-C3'	5.29	126.05	119.70
1	C1	102	G	C4-N9-C1'	5.29	133.37	126.50
3	C3	68	C	C2-N1-C1'	5.27	124.59	118.80
1	C1	1125	G	O4'-C1'-N9	5.24	112.39	108.20
23	Cz	61	MET	CA-CB-CG	5.24	122.21	113.30
1	C1	2912	U	N1-C2-O2	5.24	126.47	122.80
4	C4	50	U	N3-C2-O2	-5.23	118.54	122.20
1	C1	3132	A	P-O3'-C3'	5.23	125.97	119.70
1	C1	2584	C	C2-N1-C1'	5.23	124.55	118.80
1	C1	2730	U	C6-N1-C1'	-5.22	113.89	121.20
1	C1	168	C	C2-N1-C1'	5.21	124.53	118.80
1	C1	2544	G	C8-N9-C1'	-5.20	120.24	127.00
2	C2	113	U	C2-N1-C1'	5.20	123.94	117.70
1	C1	3016	U	N1-C2-O2	5.17	126.42	122.80
1	C1	3042	C	C6-N1-C2	-5.16	118.23	120.30
1	C1	969	U	C2-N1-C1'	5.16	123.89	117.70
1	C1	2100	U	C2-N1-C1'	5.16	123.89	117.70
1	C1	102	G	O4'-C1'-N9	5.15	112.32	108.20
1	C1	3128	A	O4'-C1'-N9	5.12	112.30	108.20
1	C1	94	C	N1-C2-O2	5.12	121.97	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C3	42	U	C2-N1-C1'	5.11	123.83	117.70
30	LH	92	LEU	CA-CB-CG	5.11	127.04	115.30
1	C1	1935	C	N1-C2-O2	5.09	121.95	118.90
1	C1	1858	G	C4-N9-C1'	5.08	133.10	126.50
1	C1	968	U	C5-C6-N1	5.08	125.24	122.70
1	C1	1851	U	N1-C2-O2	5.08	126.35	122.80
1	C1	438	C	C2-N1-C1'	5.05	124.36	118.80
1	C1	725	C	N3-C2-O2	-5.05	118.37	121.90
1	C1	1087	U	N3-C2-O2	-5.04	118.67	122.20
1	C1	2222	A	C4-N9-C1'	5.03	135.35	126.30
1	C1	831	C	C2-N1-C1'	5.02	124.32	118.80
1	C1	162	U	N1-C2-O2	5.00	126.30	122.80
1	C1	3291	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	CB	261/391 (67%)	256 (98%)	5 (2%)	0	100	100
6	CF	243/270 (90%)	238 (98%)	5 (2%)	0	100	100
7	CH	621/661 (94%)	614 (99%)	7 (1%)	0	100	100
8	CI	150/414 (36%)	149 (99%)	1 (1%)	0	100	100
9	CJ	376/679 (55%)	374 (100%)	2 (0%)	0	100	100
10	CK	231/261 (88%)	226 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	CL	77/558 (14%)	77 (100%)	0	0	100	100
12	CM	211/249 (85%)	207 (98%)	4 (2%)	0	100	100
12	LF	246/249 (99%)	240 (98%)	6 (2%)	0	100	100
13	CN	244/246 (99%)	238 (98%)	6 (2%)	0	100	100
14	CO	56/120 (47%)	56 (100%)	0	0	100	100
15	CQ	181/225 (80%)	179 (99%)	2 (1%)	0	100	100
16	Lq	137/147 (93%)	132 (96%)	5 (4%)	0	100	100
17	Cb	99/117 (85%)	98 (99%)	1 (1%)	0	100	100
18	Cd	458/627 (73%)	454 (99%)	4 (1%)	0	100	100
19	Ce	252/443 (57%)	251 (100%)	1 (0%)	0	100	100
20	Cf	281/350 (80%)	279 (99%)	2 (1%)	0	100	100
21	Cg	186/202 (92%)	186 (100%)	0	0	100	100
22	Ch	484/517 (94%)	471 (97%)	13 (3%)	0	100	100
23	Cz	99/123 (80%)	98 (99%)	1 (1%)	0	100	100
24	LA	189/254 (74%)	187 (99%)	2 (1%)	0	100	100
25	LB	387/392 (99%)	381 (98%)	6 (2%)	0	100	100
26	LC	361/365 (99%)	355 (98%)	6 (2%)	0	100	100
27	LD	282/304 (93%)	278 (99%)	4 (1%)	0	100	100
28	LE	187/200 (94%)	184 (98%)	3 (2%)	0	100	100
29	LG	233/262 (89%)	228 (98%)	5 (2%)	0	100	100
30	LH	188/229 (82%)	186 (99%)	2 (1%)	0	100	100
31	LJ	167/173 (96%)	166 (99%)	1 (1%)	0	100	100
32	LK	156/165 (94%)	155 (99%)	1 (1%)	0	100	100
33	LL	201/213 (94%)	200 (100%)	1 (0%)	0	100	100
34	LM	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
35	LN	200/203 (98%)	196 (98%)	4 (2%)	0	100	100
36	LO	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
37	LP	167/187 (89%)	164 (98%)	3 (2%)	0	100	100
38	LQ	148/213 (70%)	147 (99%)	1 (1%)	0	100	100
39	LR	153/2898 (5%)	152 (99%)	1 (1%)	0	100	100
40	LS	172/174 (99%)	170 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	LT	127/160 (79%)	126 (99%)	1 (1%)	0	100	100
42	LU	103/127 (81%)	101 (98%)	2 (2%)	0	100	100
43	LV	133/139 (96%)	132 (99%)	1 (1%)	0	100	100
44	LX	143/156 (92%)	142 (99%)	1 (1%)	0	100	100
45	LY	131/138 (95%)	128 (98%)	3 (2%)	0	100	100
46	LZ	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
47	La	104/149 (70%)	104 (100%)	0	0	100	100
48	Lc	93/108 (86%)	93 (100%)	0	0	100	100
49	Ld	108/120 (90%)	108 (100%)	0	0	100	100
50	Le	124/131 (95%)	123 (99%)	1 (1%)	0	100	100
51	Lf	106/109 (97%)	106 (100%)	0	0	100	100
52	Lg	116/119 (98%)	115 (99%)	1 (1%)	0	100	100
53	Lh	120/935 (13%)	117 (98%)	3 (2%)	0	100	100
54	Li	99/110 (90%)	99 (100%)	0	0	100	100
55	Lj	86/95 (90%)	85 (99%)	1 (1%)	0	100	100
56	Lk	74/94 (79%)	74 (100%)	0	0	100	100
57	Ll	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
58	Lp	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
All	All	10361/16395 (63%)	10225 (99%)	136 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	CB	228/329 (69%)	218 (96%)	10 (4%)	28	27
6	CF	212/236 (90%)	207 (98%)	5 (2%)	49	52
7	CH	549/575 (96%)	532 (97%)	17 (3%)	40	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CI	124/336 (37%)	120 (97%)	4 (3%)	39	40
9	CJ	331/579 (57%)	325 (98%)	6 (2%)	59	63
10	CK	206/225 (92%)	202 (98%)	4 (2%)	57	61
11	CL	61/458 (13%)	58 (95%)	3 (5%)	25	22
12	CM	185/215 (86%)	182 (98%)	3 (2%)	62	68
12	LF	213/215 (99%)	208 (98%)	5 (2%)	50	53
13	CN	205/206 (100%)	200 (98%)	5 (2%)	49	52
14	CO	48/99 (48%)	47 (98%)	1 (2%)	53	57
15	CQ	144/192 (75%)	138 (96%)	6 (4%)	30	29
16	Lq	109/112 (97%)	109 (100%)	0	100	100
17	Cb	85/101 (84%)	81 (95%)	4 (5%)	26	24
18	Cd	403/541 (74%)	393 (98%)	10 (2%)	47	50
19	Ce	223/383 (58%)	217 (97%)	6 (3%)	44	47
20	Cf	250/310 (81%)	243 (97%)	7 (3%)	43	46
21	Cg	158/176 (90%)	154 (98%)	4 (2%)	47	50
22	Ch	408/436 (94%)	396 (97%)	12 (3%)	42	44
23	Cz	89/107 (83%)	83 (93%)	6 (7%)	16	13
24	LA	150/198 (76%)	149 (99%)	1 (1%)	84	88
25	LB	329/331 (99%)	326 (99%)	3 (1%)	78	83
26	LC	282/285 (99%)	277 (98%)	5 (2%)	59	63
27	LD	221/253 (87%)	215 (97%)	6 (3%)	44	47
28	LE	157/166 (95%)	155 (99%)	2 (1%)	69	74
29	LG	200/222 (90%)	198 (99%)	2 (1%)	76	81
30	LH	167/200 (84%)	164 (98%)	3 (2%)	59	63
31	LJ	140/150 (93%)	129 (92%)	11 (8%)	12	8
32	LK	127/136 (93%)	122 (96%)	5 (4%)	32	32
33	LL	158/176 (90%)	155 (98%)	3 (2%)	57	61
34	LM	116/117 (99%)	114 (98%)	2 (2%)	60	66
35	LN	179/180 (99%)	179 (100%)	0	100	100
36	LO	162/163 (99%)	158 (98%)	4 (2%)	47	50
37	LP	133/152 (88%)	131 (98%)	2 (2%)	65	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	LQ	128/178 (72%)	124 (97%)	4 (3%)	40	42
39	LR	125/2396 (5%)	125 (100%)	0	100	100
40	LS	152/154 (99%)	148 (97%)	4 (3%)	46	49
41	LT	110/135 (82%)	107 (97%)	3 (3%)	44	47
42	LU	92/108 (85%)	90 (98%)	2 (2%)	52	55
43	LV	98/102 (96%)	96 (98%)	2 (2%)	55	59
44	LX	122/129 (95%)	117 (96%)	5 (4%)	30	30
45	LY	116/119 (98%)	107 (92%)	9 (8%)	12	9
46	LZ	121/121 (100%)	118 (98%)	3 (2%)	47	50
47	La	93/122 (76%)	91 (98%)	2 (2%)	52	55
48	Lc	76/88 (86%)	73 (96%)	3 (4%)	32	32
49	Ld	90/105 (86%)	90 (100%)	0	100	100
50	Le	109/114 (96%)	108 (99%)	1 (1%)	78	83
51	Lf	89/90 (99%)	89 (100%)	0	100	100
52	Lg	95/102 (93%)	94 (99%)	1 (1%)	73	79
53	Lh	109/781 (14%)	108 (99%)	1 (1%)	78	83
54	Li	85/93 (91%)	84 (99%)	1 (1%)	71	77
55	Lj	72/78 (92%)	69 (96%)	3 (4%)	30	29
56	Lk	73/88 (83%)	67 (92%)	6 (8%)	11	7
57	Ll	45/46 (98%)	44 (98%)	1 (2%)	52	55
58	Lp	73/74 (99%)	70 (96%)	3 (4%)	30	30
All	All	8825/13783 (64%)	8604 (98%)	221 (2%)	50	50

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	CB	36	LYS
5	CB	70	LYS
5	CB	77	ARG
5	CB	106	ARG
5	CB	185	MET
5	CB	210	GLU
5	CB	279	ARG
5	CB	281	PHE
5	CB	284	LYS

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Mol	Chain	Res	Type
5	CB	297	ASP
6	CF	5	LYS
6	CF	8	ARG
6	CF	64	ARG
6	CF	231	SER
6	CF	246	ARG
7	CH	79	ASP
7	CH	85	TYR
7	CH	128	LYS
7	CH	140	LYS
7	CH	168	THR
7	CH	246	ARG
7	CH	264	LYS
7	CH	300	GLU
7	CH	318	ARG
7	CH	325	GLU
7	CH	344	SER
7	CH	348	LYS
7	CH	379	ARG
7	CH	388	LYS
7	CH	395	LYS
7	CH	469	GLU
7	CH	490	GLN
8	CI	198	PHE
8	CI	278	ARG
8	CI	295	ARG
8	CI	318	GLU
9	CJ	67	LYS
9	CJ	115	LYS
9	CJ	364	SER
9	CJ	381	GLN
9	CJ	393	LYS
9	CJ	469	GLU
10	CK	98	THR
10	CK	144	LYS
10	CK	185	THR
10	CK	190	ASN
11	CL	41	LYS
11	CL	67	GLN
11	CL	73	ARG
12	CM	31	GLU
12	CM	178	ASN

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Mol	Chain	Res	Type
12	CM	230	GLU
13	CN	51	THR
13	CN	61	ARG
13	CN	91	ASP
13	CN	168	GLN
13	CN	188	ARG
14	CO	110	MET
15	CQ	57	LYS
15	CQ	63	MET
15	CQ	88	LYS
15	CQ	136	ARG
15	CQ	163	GLU
15	CQ	173	SER
17	Cb	18	ASP
17	Cb	28	SER
17	Cb	39	LYS
17	Cb	68	HIS
18	Cd	86	ASP
18	Cd	129	LYS
18	Cd	133	LYS
18	Cd	181	GLU
18	Cd	219	SER
18	Cd	278	SER
18	Cd	364	TRP
18	Cd	430	ARG
18	Cd	433	LYS
18	Cd	458	ASP
19	Ce	102	SER
19	Ce	184	LYS
19	Ce	224	GLN
19	Ce	231	GLU
19	Ce	369	LYS
19	Ce	387	ASP
20	Cf	93	ASN
20	Cf	139	ARG
20	Cf	166	ASP
20	Cf	261	ARG
20	Cf	280	GLU
20	Cf	281	GLU
20	Cf	319	ARG
21	Cg	19	THR
21	Cg	49	GLN

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Mol	Chain	Res	Type
21	Cg	56	ARG
21	Cg	71	THR
22	Ch	45	ASP
22	Ch	86	ARG
22	Ch	97	ASP
22	Ch	152	CYS
22	Ch	219	GLU
22	Ch	222	LYS
22	Ch	285	CYS
22	Ch	292	ASP
22	Ch	351	GLU
22	Ch	366	LYS
22	Ch	370	LYS
22	Ch	426	ASN
23	Cz	22	ASN
23	Cz	86	ARG
23	Cz	87	ARG
23	Cz	95	ARG
23	Cz	97	GLU
23	Cz	98	GLN
24	LA	114	SER
25	LB	66	LYS
25	LB	168	ARG
25	LB	197	ARG
26	LC	121	PHE
26	LC	198	MET
26	LC	270	GLU
26	LC	289	ARG
26	LC	338	LYS
27	LD	34	LYS
27	LD	50	ARG
27	LD	51	LEU
27	LD	95	TRP
27	LD	129	TYR
27	LD	155	ARG
28	LE	6	THR
28	LE	155	SER
12	LF	23	LYS
12	LF	31	GLU
12	LF	38	LYS
12	LF	62	ARG
12	LF	246	ARG

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Mol	Chain	Res	Type
29	LG	216	LYS
29	LG	246	GLN
30	LH	56	SER
30	LH	85	VAL
30	LH	100	LYS
31	LJ	14	ARG
31	LJ	45	THR
31	LJ	62	ARG
31	LJ	86	LYS
31	LJ	93	ARG
31	LJ	94	ARG
31	LJ	95	ARG
31	LJ	112	ASP
31	LJ	117	TYR
31	LJ	127	ASP
31	LJ	166	GLN
32	LK	15	LEU
32	LK	40	LYS
32	LK	68	GLN
32	LK	91	ASP
32	LK	93	LYS
33	LL	135	LYS
33	LL	140	LYS
33	LL	183	ARG
34	LM	5	ASN
34	LM	35	ASP
36	LO	76	ARG
36	LO	80	ARG
36	LO	194	LYS
36	LO	196	SER
37	LP	55	LYS
37	LP	169	SER
38	LQ	35	ARG
38	LQ	41	SER
38	LQ	69	GLU
38	LQ	126	MET
40	LS	1	MET
40	LS	84	ARG
40	LS	115	ARG
40	LS	119	ARG
41	LT	72	VAL
41	LT	114	GLU

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Mol	Chain	Res	Type
41	LT	127	GLN
42	LU	30	SER
42	LU	106	SER
43	LV	74	LYS
43	LV	98	GLU
44	LX	37	THR
44	LX	66	HIS
44	LX	69	ARG
44	LX	71	ASP
44	LX	83	GLU
45	LY	2	LYS
45	LY	37	GLU
45	LY	46	SER
45	LY	54	GLU
45	LY	68	LYS
45	LY	73	TYR
45	LY	78	VAL
45	LY	88	LYS
45	LY	114	ARG
46	LZ	33	LYS
46	LZ	58	LYS
46	LZ	60	ARG
47	La	85	ASP
47	La	92	SER
48	Lc	67	LYS
48	Lc	93	MET
48	Lc	101	SER
50	Le	124	LYS
52	Lg	87	ARG
53	Lh	19	GLU
54	Li	105	GLU
55	Lj	6	SER
55	Lj	7	SER
55	Lj	65	ARG
56	Lk	7	ASP
56	Lk	10	LYS
56	Lk	24	ARG
56	Lk	33	GLN
56	Lk	51	ASP
56	Lk	70	ASP
57	Ll	45	ARG
58	Lp	11	SER

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Mol	Chain	Res	Type
58	Lp	56	SER
58	Lp	72	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
32	LK	65	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	3069/3342 (91%)	550 (17%)	23 (0%)
2	C2	155/156 (99%)	21 (13%)	0
3	C3	80/162 (49%)	21 (26%)	0
4	C4	118/119 (99%)	23 (19%)	0
All	All	3422/3779 (90%)	615 (17%)	23 (0%)

All (615) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	4	U
1	C1	6	G
1	C1	27	A
1	C1	44	A
1	C1	50	A
1	C1	60	G
1	C1	61	A
1	C1	66	A
1	C1	67	A
1	C1	75	G
1	C1	95	G
1	C1	96	A
1	C1	110	A
1	C1	111	G
1	C1	112	C
1	C1	116	A
1	C1	117	A
1	C1	119	U
1	C1	123	A
1	C1	132	U

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Mol	Chain	Res	Type
1	C1	134	G
1	C1	135	G
1	C1	139	G
1	C1	151	G
1	C1	152	G
1	C1	153	A
1	C1	157	G
1	C1	181	G
1	C1	184	U
1	C1	185	U
1	C1	193	A
1	C1	204	C
1	C1	213	A
1	C1	214	G
1	C1	225	A
1	C1	241	U
1	C1	244	G
1	C1	247	A
1	C1	258	A
1	C1	262	G
1	C1	276	G
1	C1	277	A
1	C1	288	A
1	C1	291	U
1	C1	298	U
1	C1	308	C
1	C1	316	A
1	C1	322	C
1	C1	323	G
1	C1	332	C
1	C1	342	A
1	C1	343	C
1	C1	369	G
1	C1	389	A2M
1	C1	391	U
1	C1	394	C
1	C1	395	A
1	C1	396	C
1	C1	414	G
1	C1	415	A
1	C1	434	U
1	C1	435	G

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Mol	Chain	Res	Type
1	C1	443	C
1	C1	445	G
1	C1	446	A
1	C1	447	U
1	C1	448	C
1	C1	458	U
1	C1	459	C
1	C1	460	U
1	C1	469	C
1	C1	470	A
1	C1	471	C
1	C1	472	U
1	C1	479	G
1	C1	485	G
1	C1	512	A
1	C1	514	A
1	C1	524	A
1	C1	527	G
1	C1	536	C
1	C1	537	C
1	C1	545	U
1	C1	547	A
1	C1	548	U
1	C1	549	A
1	C1	550	G
1	C1	570	G
1	C1	583	A
1	C1	588	G
1	C1	592	U
1	C1	593	G
1	C1	595	A
1	C1	597	G
1	C1	599	A
1	C1	608	U
1	C1	609	A
1	C1	610	A
1	C1	624	C
1	C1	632	G
1	C1	634	A
1	C1	648	A
1	C1	650	U
1	C1	665	A

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Mol	Chain	Res	Type
1	C1	669	U
1	C1	678	A
1	C1	693	A
1	C1	700	G
1	C1	703	A
1	C1	704	A
1	C1	719	U
1	C1	720	C
1	C1	721	G
1	C1	747	A
1	C1	748	U
1	C1	757	A
1	C1	759	U
1	C1	761	G
1	C1	762	A
1	C1	763	G
1	C1	766	G
1	C1	767	G
1	C1	782	G
1	C1	790	A
1	C1	799	A
1	C1	808	G
1	C1	812	A
1	C1	830	A
1	C1	843	C
1	C1	857	G
1	C1	877	A
1	C1	879	U
1	C1	889	G
1	C1	896	A
1	C1	898	G
1	C1	899	A
1	C1	903	A
1	C1	906	G
1	C1	919	G
1	C1	926	A
1	C1	931	C
1	C1	933	A
1	C1	934	A
1	C1	935	G
1	C1	937	U
1	C1	940	C

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Mol	Chain	Res	Type
1	C1	941	C
1	C1	944	A
1	C1	945	G
1	C1	947	A
1	C1	954	U
1	C1	955	G
1	C1	956	U
1	C1	963	U
1	C1	964	C
1	C1	966	G
1	C1	976	G
1	C1	977	U
1	C1	983	G
1	C1	984	A
1	C1	1032	C
1	C1	1034	U
1	C1	1040	A
1	C1	1047	A
1	C1	1048	A
1	C1	1049	G
1	C1	1051	C
1	C1	1055	G
1	C1	1058	A
1	C1	1059	C
1	C1	1064	C
1	C1	1065	U
1	C1	1066	G
1	C1	1070	G
1	C1	1075	C
1	C1	1076	A
1	C1	1077	U
1	C1	1078	U
1	C1	1079	C
1	C1	1080	G
1	C1	1081	A
1	C1	1086	A
1	C1	1098	G
1	C1	1099	G
1	C1	1109	G
1	C1	1110	G
1	C1	1115	C
1	C1	1118	A

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Mol	Chain	Res	Type
1	C1	1127	U
1	C1	1132	G
1	C1	1136	A
1	C1	1143	C
1	C1	1161	G
1	C1	1163	G
1	C1	1164	U
1	C1	1165	G
1	C1	1173	A
1	C1	1175	C
1	C1	1176	A
1	C1	1179	C
1	C1	1185	A
1	C1	1187	A
1	C1	1194	U
1	C1	1205	G
1	C1	1209	G
1	C1	1228	A
1	C1	1241	U
1	C1	1246	A
1	C1	1248	U
1	C1	1255	C
1	C1	1268	G
1	C1	1278	G
1	C1	1287	A
1	C1	1288	U
1	C1	1290	G
1	C1	1292	U
1	C1	1296	G
1	C1	1313	A
1	C1	1331	A
1	C1	1332	G
1	C1	1333	A
1	C1	1334	A
1	C1	1335	A
1	C1	1336	C
1	C1	1337	G
1	C1	1370	G
1	C1	1382	A
1	C1	1383	G
1	C1	1417	G
1	C1	1420	OMC

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Mol	Chain	Res	Type
1	C1	1429	A
1	C1	1433	OMG
1	C1	1438	U
1	C1	1458	G
1	C1	1464	A
1	C1	1485	G
1	C1	1491	OMC
1	C1	1505	U
1	C1	1536	U
1	C1	1538	U
1	C1	1539	C
1	C1	1540	A
1	C1	1542	A
1	C1	1543	G
1	C1	1549	C
1	C1	1550	U
1	C1	1554	G
1	C1	1560	U
1	C1	1561	G
1	C1	1563	G
1	C1	1567	A
1	C1	1568	A
1	C1	1569	A
1	C1	1573	A
1	C1	1576	C
1	C1	1585	A
1	C1	1586	U
1	C1	1609	U
1	C1	1619	C
1	C1	1622	A
1	C1	1623	A
1	C1	1624	C
1	C1	1663	C
1	C1	1683	U
1	C1	1685	U
1	C1	1697	C
1	C1	1704	U
1	C1	1705	C
1	C1	1722	U
1	C1	1730	A
1	C1	1731	G
1	C1	1743	U

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Mol	Chain	Res	Type
1	C1	1745	U
1	C1	1746	G
1	C1	1751	G
1	C1	1760	G
1	C1	1776	G
1	C1	1777	A
1	C1	1792	G
1	C1	1793	A
1	C1	1794	A
1	C1	1795	U
1	C1	1796	A
1	C1	1799	U
1	C1	1800	C
1	C1	1801	U
1	C1	1822	A
1	C1	1826	C
1	C1	1829	C
1	C1	1846	C
1	C1	1847	A2M
1	C1	1856	U
1	C1	1858	G
1	C1	1860	U
1	C1	1866	A
1	C1	1886	G
1	C1	1887	C
1	C1	1917	OMU
1	C1	1923	C
1	C1	1934	G
1	C1	1935	C
1	C1	1937	C
1	C1	2046	C
1	C1	2048	U
1	C1	2050	C
1	C1	2052	G
1	C1	2054	U
1	C1	2056	A
1	C1	2076	A
1	C1	2084	G
1	C1	2085	G
1	C1	2089	A
1	C1	2094	A
1	C1	2103	U

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Mol	Chain	Res	Type
1	C1	2121	A
1	C1	2126	C
1	C1	2132	G
1	C1	2151	A
1	C1	2156	U
1	C1	2157	G
1	C1	2158	C
1	C1	2161	A
1	C1	2167	C
1	C1	2168	U
1	C1	2169	G
1	C1	2171	A
1	C1	2172	U
1	C1	2186	A
1	C1	2188	U
1	C1	2192	A
1	C1	2203	G
1	C1	2205	A
1	C1	2206	A
1	C1	2212	G
1	C1	2216	G
1	C1	2217	U
1	C1	2218	A
1	C1	2219	A
1	C1	2220	C
1	C1	2221	U
1	C1	2222	A
1	C1	2223	U
1	C1	2224	G
1	C1	2225	A
1	C1	2226	C
1	C1	2229	U
1	C1	2230	C
1	C1	2231	U
1	C1	2237	U
1	C1	2279	G
1	C1	2281	U
1	C1	2282	U
1	C1	2284	A
1	C1	2297	U
1	C1	2298	G
1	C1	2299	U

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Mol	Chain	Res	Type
1	C1	2326	A
1	C1	2340	G
1	C1	2348	A
1	C1	2351	U
1	C1	2355	C
1	C1	2356	G
1	C1	2362	A
1	C1	2364	A
1	C1	2373	U
1	C1	2374	U
1	C1	2381	G
1	C1	2382	A
1	C1	2398	G
1	C1	2403	A
1	C1	2406	A
1	C1	2473	U
1	C1	2474	A
1	C1	2477	U
1	C1	2489	C
1	C1	2499	C
1	C1	2501	U
1	C1	2502	G
1	C1	2503	C
1	C1	2506	C
1	C1	2507	C
1	C1	2508	A
1	C1	2515	G
1	C1	2516	G
1	C1	2521	A
1	C1	2527	C
1	C1	2533	G
1	C1	2544	G
1	C1	2545	G
1	C1	2552	A
1	C1	2565	G
1	C1	2566	G
1	C1	2573	G
1	C1	2575	C
1	C1	2576	U
1	C1	2577	G
1	C1	2578	OMG
1	C1	2582	G

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Mol	Chain	Res	Type
1	C1	2584	C
1	C1	2585	A
1	C1	2609	U
1	C1	2615	A
1	C1	2633	A
1	C1	2635	A
1	C1	2636	G
1	C1	2647	U
1	C1	2650	A
1	C1	2651	A
1	C1	2656	A
1	C1	2657	G
1	C1	2663	A
1	C1	2664	A
1	C1	2667	C
1	C1	2672	U
1	C1	2673	G
1	C1	2674	A
1	C1	2675	U
1	C1	2680	A
1	C1	2689	G
1	C1	2690	OMU
1	C1	2691	G
1	C1	2713	G
1	C1	2717	A
1	C1	2730	U
1	C1	2731	C
1	C1	2732	C
1	C1	2736	G
1	C1	2737	A
1	C1	2754	U
1	C1	2755	G
1	C1	2756	C
1	C1	2757	C
1	C1	2758	A
1	C1	2761	A
1	C1	2762	A
1	C1	2763	A
1	C1	2769	C
1	C1	2773	G
1	C1	2783	G
1	C1	2784	C

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Mol	Chain	Res	Type
1	C1	2785	U
1	C1	2802	U
1	C1	2803	C
1	C1	2805	U
1	C1	2806	A
1	C1	2808	C
1	C1	2812	G
1	C1	2816	C
1	C1	2817	U
1	C1	2826	C
1	C1	2828	U
1	C1	2836	G
1	C1	2846	A
1	C1	2857	G
1	C1	2858	C
1	C1	2863	U
1	C1	2882	U
1	C1	2883	U
1	C1	2884	C
1	C1	2885	A
1	C1	2887	C
1	C1	2894	U
1	C1	2895	A
1	C1	2903	U
1	C1	2905	A
1	C1	2929	C
1	C1	2930	A
1	C1	2931	G
1	C1	2938	U
1	C1	2939	U
1	C1	2940	U
1	C1	2942	C
1	C1	2949	G
1	C1	2951	U
1	C1	2955	C
1	C1	2956	U
1	C1	2970	A
1	C1	2980	G
1	C1	3014	U
1	C1	3017	G
1	C1	3036	G
1	C1	3044	A

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Mol	Chain	Res	Type
1	C1	3050	C
1	C1	3051	C
1	C1	3067	G
1	C1	3071	A
1	C1	3080	A
1	C1	3086	G
1	C1	3087	A
1	C1	3088	A
1	C1	3089	U
1	C1	3100	A
1	C1	3101	C
1	C1	3102	G
1	C1	3112	U
1	C1	3113	A
1	C1	3119	A
1	C1	3124	G
1	C1	3125	U
1	C1	3126	A
1	C1	3127	G
1	C1	3131	U
1	C1	3133	U
1	C1	3135	A
1	C1	3141	G
1	C1	3146	C
1	C1	3155	A
1	C1	3162	C
1	C1	3163	A
1	C1	3164	G
1	C1	3168	A
1	C1	3185	G
1	C1	3186	A
1	C1	3188	G
1	C1	3190	G
1	C1	3200	A
1	C1	3206	C
1	C1	3210	U
1	C1	3211	U
1	C1	3214	A
1	C1	3217	U
1	C1	3218	U
1	C1	3228	C
1	C1	3229	G

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Mol	Chain	Res	Type
1	C1	3231	G
1	C1	3245	C
1	C1	3248	A
1	C1	3254	U
1	C1	3257	A
1	C1	3258	U
1	C1	3259	G
1	C1	3260	U
1	C1	3282	U
1	C1	3286	G
1	C1	3292	U
1	C1	3293	U
1	C1	3295	U
1	C1	3297	G
1	C1	3299	U
1	C1	3302	G
1	C1	3310	G
1	C1	3312	G
1	C1	3316	A
1	C1	3319	C
1	C1	3323	C
1	C1	3324	C
1	C1	3325	U
1	C1	3331	U
1	C1	3332	A
1	C1	3338	C
2	C2	34	U
2	C2	35	C
2	C2	52	A
2	C2	59	A
2	C2	62	A
2	C2	63	G
2	C2	81	U
2	C2	82	U
2	C2	83	C
2	C2	84	C
2	C2	87	G
2	C2	90	U
2	C2	95	G
2	C2	104	A
2	C2	106	C
2	C2	113	U

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Mol	Chain	Res	Type
2	C2	116	G
2	C2	125	U
2	C2	127	U
2	C2	151	C
2	C2	154	C
3	C3	2	U
3	C3	3	C
3	C3	10	C
3	C3	19	G
3	C3	20	G
3	C3	25	U
3	C3	36	C
3	C3	39	G
3	C3	40	G
3	C3	42	U
3	C3	57	A
3	C3	58	A
3	C3	59	A
3	C3	63	A
3	C3	66	G
3	C3	68	C
3	C3	69	G
3	C3	135	G
3	C3	136	C
3	C3	137	C
3	C3	138	A
4	C4	6	C
4	C4	7	G
4	C4	42	C
4	C4	52	G
4	C4	54	U
4	C4	55	A
4	C4	64	A
4	C4	66	G
4	C4	75	A
4	C4	76	G
4	C4	78	A
4	C4	82	G
4	C4	83	G
4	C4	84	G
4	C4	85	U
4	C4	86	C

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Mol	Chain	Res	Type
4	C4	89	U
4	C4	90	G
4	C4	93	G
4	C4	97	A
4	C4	98	G
4	C4	101	A
4	C4	111	G

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	151	G
1	C1	243	U
1	C1	898	G
1	C1	1047	A
1	C1	1064	C
1	C1	1077	U
1	C1	1267	C
1	C1	1537	U
1	C1	2157	G
1	C1	2160	C
1	C1	2225	A
1	C1	2280	A
1	C1	2575	C
1	C1	2883	U
1	C1	3079	U
1	C1	3132	A
1	C1	3205	G
1	C1	3210	U
1	C1	3230	G
1	C1	3258	U
1	C1	3298	U
1	C1	3301	C
1	C1	3324	C

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

34 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMG	C1	646	1	18,26,27	1.22	2 (11%)	19,38,41	0.87	2 (10%)
1	A2M	C1	637	1	18,25,26	4.30	7 (38%)	18,36,39	3.94	4 (22%)
1	OMG	C1	627	1	18,26,27	1.24	3 (16%)	19,38,41	0.99	1 (5%)
1	OMC	C1	778	1	19,22,23	0.59	0	26,31,34	0.85	1 (3%)
1	A2M	C1	858	1	18,25,26	4.38	8 (44%)	18,36,39	3.98	4 (22%)
1	A2M	C1	1223	1	18,25,26	4.28	8 (44%)	18,36,39	3.88	5 (27%)
1	OMU	C1	2277	1	19,22,23	2.99	6 (31%)	26,31,34	1.69	4 (15%)
1	OMG	C1	2774	1	18,26,27	1.21	2 (11%)	19,38,41	0.86	1 (5%)
1	OMG	C1	2881	1	18,26,27	1.16	2 (11%)	19,38,41	0.84	1 (5%)
1	OMC	C1	1836	1	19,22,23	0.63	0	26,31,34	0.70	0
1	OMU	C1	2688	1	19,22,23	2.99	6 (31%)	26,31,34	1.67	4 (15%)
1	OMU	C1	1868	1	19,22,23	2.98	7 (36%)	26,31,34	1.88	5 (19%)
1	A2M	C1	389	1	18,25,26	4.33	8 (44%)	18,36,39	3.87	4 (22%)
1	OMC	C1	1491	1	19,22,23	0.62	0	26,31,34	0.70	0
1	OMU	C1	2690	1	19,22,23	2.98	7 (36%)	26,31,34	1.74	4 (15%)
1	OMC	C1	2918	1	19,22,23	0.64	0	26,31,34	0.78	0
1	OMG	C1	385	1	18,26,27	1.19	2 (11%)	19,38,41	0.80	1 (5%)
1	OMG	C1	1433	1	18,26,27	1.24	2 (11%)	19,38,41	0.86	1 (5%)
1	OMG	C1	2876	1	18,26,27	1.16	2 (11%)	19,38,41	0.88	1 (5%)
1	A2M	C1	1432	1	18,25,26	4.33	8 (44%)	18,36,39	3.94	4 (22%)
1	OMU	C1	1917	1	19,22,23	3.01	6 (31%)	26,31,34	1.75	6 (23%)
1	OMC	C1	2838	1	19,22,23	0.77	1 (5%)	26,31,34	1.54	4 (15%)
1	OMC	C1	1812	1	19,22,23	0.64	0	26,31,34	1.38	2 (7%)
1	OMU	C1	2380	1	19,22,23	2.96	7 (36%)	26,31,34	1.69	5 (19%)
1	OMC	C1	1420	1	19,22,23	0.71	0	26,31,34	1.24	3 (11%)
1	OMC	C1	2300	1	19,22,23	0.62	0	26,31,34	0.66	0
1	A2M	C1	2289	1	18,25,26	4.37	7 (38%)	18,36,39	3.77	4 (22%)
1	A2M	C1	1847	1	18,25,26	4.33	8 (44%)	18,36,39	4.01	5 (27%)
1	OMG	C1	2578	1	18,26,27	1.20	2 (11%)	19,38,41	0.99	1 (5%)
1	OMG	C1	787	1	18,26,27	1.20	2 (11%)	19,38,41	0.92	1 (5%)
1	OMU	C1	2683	1	19,22,23	2.96	7 (36%)	26,31,34	1.73	5 (19%)
1	OMU	C1	2384	1	19,22,23	3.02	7 (36%)	26,31,34	1.71	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	A2M	C1	848	1	18,25,26	4.34	9 (50%)	18,36,39	3.83	5 (27%)
1	OMG	C1	2358	1	18,26,27	1.21	2 (11%)	19,38,41	0.85	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	C1	646	1	-	0/5/27/28	0/3/3/3
1	A2M	C1	637	1	-	1/5/27/28	0/3/3/3
1	OMG	C1	627	1	-	0/5/27/28	0/3/3/3
1	OMC	C1	778	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	858	1	-	0/5/27/28	0/3/3/3
1	A2M	C1	1223	1	-	1/5/27/28	0/3/3/3
1	OMU	C1	2277	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	2774	1	-	0/5/27/28	0/3/3/3
1	OMG	C1	2881	1	-	0/5/27/28	0/3/3/3
1	OMC	C1	1836	1	-	0/9/27/28	0/2/2/2
1	OMU	C1	2688	1	-	0/9/27/28	0/2/2/2
1	OMU	C1	1868	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	389	1	-	3/5/27/28	0/3/3/3
1	OMC	C1	1491	1	-	1/9/27/28	0/2/2/2
1	OMU	C1	2690	1	-	2/9/27/28	0/2/2/2
1	OMC	C1	2918	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	385	1	-	2/5/27/28	0/3/3/3
1	OMG	C1	1433	1	-	3/5/27/28	0/3/3/3
1	OMG	C1	2876	1	-	0/5/27/28	0/3/3/3
1	A2M	C1	1432	1	-	0/5/27/28	0/3/3/3
1	OMU	C1	1917	1	-	2/9/27/28	0/2/2/2
1	OMC	C1	2838	1	-	2/9/27/28	0/2/2/2
1	OMC	C1	1812	1	-	2/9/27/28	0/2/2/2
1	OMU	C1	2380	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	1420	1	-	4/9/27/28	0/2/2/2
1	OMC	C1	2300	1	-	1/9/27/28	0/2/2/2
1	A2M	C1	2289	1	-	0/5/27/28	0/3/3/3
1	A2M	C1	1847	1	-	3/5/27/28	0/3/3/3
1	OMG	C1	2578	1	-	3/5/27/28	0/3/3/3
1	OMG	C1	787	1	-	0/5/27/28	0/3/3/3
1	OMU	C1	2683	1	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	C1	2384	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	848	1	-	0/5/27/28	0/3/3/3
1	OMG	C1	2358	1	-	0/5/27/28	0/3/3/3

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2289	A2M	C3'-C2'	-12.93	1.24	1.52
1	C1	858	A2M	C3'-C2'	-12.83	1.24	1.52
1	C1	637	A2M	C3'-C2'	-12.72	1.24	1.52
1	C1	1223	A2M	C3'-C2'	-12.71	1.24	1.52
1	C1	1432	A2M	C3'-C2'	-12.66	1.24	1.52
1	C1	1847	A2M	C3'-C2'	-12.66	1.24	1.52
1	C1	848	A2M	C3'-C2'	-12.66	1.24	1.52
1	C1	389	A2M	C3'-C2'	-12.56	1.24	1.52
1	C1	1847	A2M	O4'-C1'	8.04	1.52	1.41
1	C1	848	A2M	O4'-C1'	7.99	1.52	1.41
1	C1	2289	A2M	O4'-C1'	7.99	1.52	1.41
1	C1	858	A2M	O4'-C1'	7.94	1.52	1.41
1	C1	1432	A2M	O4'-C1'	7.93	1.52	1.41
1	C1	389	A2M	O4'-C1'	7.73	1.51	1.41
1	C1	637	A2M	O4'-C1'	7.58	1.51	1.41
1	C1	1917	OMU	C2-N1	7.45	1.50	1.38
1	C1	1223	A2M	O4'-C1'	7.34	1.51	1.41
1	C1	1868	OMU	C2-N1	7.27	1.50	1.38
1	C1	2384	OMU	C2-N1	7.25	1.50	1.38
1	C1	2277	OMU	C2-N1	7.06	1.49	1.38
1	C1	2690	OMU	C2-N1	7.06	1.49	1.38
1	C1	2688	OMU	C2-N1	7.05	1.49	1.38
1	C1	2277	OMU	C2-N3	6.99	1.50	1.38
1	C1	2683	OMU	C2-N1	6.98	1.49	1.38
1	C1	2384	OMU	C2-N3	6.97	1.50	1.38
1	C1	2688	OMU	C2-N3	6.95	1.50	1.38
1	C1	2380	OMU	C2-N1	6.91	1.49	1.38
1	C1	2683	OMU	C2-N3	6.88	1.50	1.38
1	C1	2690	OMU	C2-N3	6.86	1.50	1.38
1	C1	2380	OMU	C2-N3	6.83	1.50	1.38
1	C1	1868	OMU	C2-N3	6.77	1.50	1.38
1	C1	1917	OMU	C2-N3	6.76	1.50	1.38
1	C1	389	A2M	O4'-C4'	-6.73	1.29	1.45
1	C1	637	A2M	O4'-C4'	-6.60	1.30	1.45
1	C1	1847	A2M	O4'-C4'	-6.58	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	1432	A2M	O4'-C4'	-6.54	1.30	1.45
1	C1	858	A2M	O4'-C4'	-6.50	1.30	1.45
1	C1	1223	A2M	O4'-C4'	-6.47	1.30	1.45
1	C1	848	A2M	O4'-C4'	-6.30	1.30	1.45
1	C1	2289	A2M	O4'-C4'	-6.29	1.30	1.45
1	C1	2380	OMU	C6-C5	6.11	1.49	1.35
1	C1	1917	OMU	C6-C5	6.09	1.49	1.35
1	C1	2688	OMU	C6-C5	6.06	1.49	1.35
1	C1	2277	OMU	C6-C5	6.03	1.49	1.35
1	C1	1868	OMU	C6-C5	6.00	1.49	1.35
1	C1	2384	OMU	C6-C5	5.99	1.49	1.35
1	C1	2690	OMU	C6-C5	5.98	1.49	1.35
1	C1	2683	OMU	C6-C5	5.91	1.48	1.35
1	C1	848	A2M	C3'-C4'	5.36	1.66	1.53
1	C1	858	A2M	C3'-C4'	5.34	1.66	1.53
1	C1	2289	A2M	C3'-C4'	5.29	1.66	1.53
1	C1	1432	A2M	C3'-C4'	5.26	1.66	1.53
1	C1	1223	A2M	C3'-C4'	5.22	1.66	1.53
1	C1	389	A2M	C3'-C4'	4.98	1.65	1.53
1	C1	637	A2M	C3'-C4'	4.98	1.65	1.53
1	C1	1847	A2M	C3'-C4'	4.86	1.65	1.53
1	C1	2384	OMU	C4-N3	4.16	1.46	1.38
1	C1	2683	OMU	C4-N3	4.10	1.45	1.38
1	C1	2277	OMU	C4-N3	4.07	1.45	1.38
1	C1	2688	OMU	C4-N3	4.04	1.45	1.38
1	C1	2690	OMU	C4-N3	3.87	1.45	1.38
1	C1	2380	OMU	C4-N3	3.85	1.45	1.38
1	C1	389	A2M	O2'-C2'	3.76	1.52	1.42
1	C1	1917	OMU	C4-N3	3.74	1.45	1.38
1	C1	1868	OMU	C4-N3	3.71	1.45	1.38
1	C1	848	A2M	O2'-C2'	3.43	1.51	1.42
1	C1	858	A2M	O2'-C2'	3.43	1.51	1.42
1	C1	1223	A2M	O2'-C2'	3.41	1.51	1.42
1	C1	637	A2M	O2'-C2'	3.41	1.51	1.42
1	C1	2289	A2M	O2'-C2'	3.41	1.51	1.42
1	C1	1847	A2M	O2'-C2'	3.40	1.51	1.42
1	C1	1432	A2M	O2'-C2'	3.39	1.51	1.42
1	C1	1433	OMG	C8-N7	-3.27	1.29	1.35
1	C1	646	OMG	C8-N7	-3.16	1.29	1.35
1	C1	627	OMG	C8-N7	-3.16	1.29	1.35
1	C1	787	OMG	C8-N7	-3.13	1.29	1.35
1	C1	2578	OMG	C8-N7	-3.11	1.29	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	858	A2M	C6-N6	3.08	1.45	1.34
1	C1	637	A2M	C6-N6	3.04	1.45	1.34
1	C1	2358	OMG	C8-N7	-3.04	1.29	1.35
1	C1	848	A2M	C6-N6	3.04	1.45	1.34
1	C1	2289	A2M	C6-N6	3.03	1.45	1.34
1	C1	1432	A2M	C6-N6	3.02	1.45	1.34
1	C1	1847	A2M	C6-N6	3.01	1.45	1.34
1	C1	389	A2M	C6-N6	3.00	1.45	1.34
1	C1	1223	A2M	C6-N6	3.00	1.45	1.34
1	C1	2881	OMG	C8-N7	-3.00	1.29	1.35
1	C1	385	OMG	C8-N7	-3.00	1.29	1.35
1	C1	2774	OMG	C8-N7	-2.93	1.30	1.35
1	C1	2876	OMG	C8-N7	-2.93	1.30	1.35
1	C1	858	A2M	C5-C4	-2.87	1.33	1.40
1	C1	2289	A2M	C5-C4	-2.84	1.33	1.40
1	C1	389	A2M	C5-C4	-2.83	1.33	1.40
1	C1	1223	A2M	C5-C4	-2.79	1.33	1.40
1	C1	848	A2M	C5-C4	-2.79	1.33	1.40
1	C1	637	A2M	C5-C4	-2.78	1.33	1.40
1	C1	1432	A2M	C5-C4	-2.77	1.33	1.40
1	C1	1847	A2M	C5-C4	-2.73	1.33	1.40
1	C1	2380	OMU	C6-N1	2.66	1.44	1.38
1	C1	2688	OMU	C6-N1	2.61	1.44	1.38
1	C1	1917	OMU	C6-N1	2.59	1.44	1.38
1	C1	1868	OMU	C6-N1	2.59	1.44	1.38
1	C1	2277	OMU	C6-N1	2.58	1.44	1.38
1	C1	646	OMG	C5-C6	-2.57	1.42	1.47
1	C1	2384	OMU	C6-N1	2.55	1.44	1.38
1	C1	1433	OMG	C5-C6	-2.53	1.42	1.47
1	C1	2690	OMU	C6-N1	2.53	1.44	1.38
1	C1	787	OMG	C5-C6	-2.49	1.42	1.47
1	C1	2358	OMG	C5-C6	-2.48	1.42	1.47
1	C1	385	OMG	C5-C6	-2.46	1.42	1.47
1	C1	2683	OMU	C6-N1	2.44	1.43	1.38
1	C1	627	OMG	C5-C6	-2.41	1.42	1.47
1	C1	2774	OMG	C5-C6	-2.41	1.42	1.47
1	C1	2881	OMG	C5-C6	-2.37	1.42	1.47
1	C1	2876	OMG	C5-C6	-2.37	1.42	1.47
1	C1	2578	OMG	C5-C6	-2.37	1.42	1.47
1	C1	848	A2M	O3'-C3'	2.21	1.48	1.43
1	C1	1868	OMU	C5-C4	2.15	1.48	1.43
1	C1	1847	A2M	O3'-C3'	2.15	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	1917	OMU	C5-C4	2.14	1.48	1.43
1	C1	2683	OMU	C5-C4	2.12	1.48	1.43
1	C1	2380	OMU	C5-C4	2.12	1.48	1.43
1	C1	2688	OMU	C5-C4	2.11	1.48	1.43
1	C1	2690	OMU	C5-C4	2.10	1.48	1.43
1	C1	858	A2M	O3'-C3'	2.10	1.47	1.43
1	C1	848	A2M	C2-N3	2.10	1.35	1.32
1	C1	1223	A2M	O3'-C3'	2.08	1.47	1.43
1	C1	2683	OMU	O4-C4	-2.08	1.20	1.24
1	C1	2277	OMU	C5-C4	2.08	1.48	1.43
1	C1	389	A2M	O3'-C3'	2.08	1.47	1.43
1	C1	1432	A2M	O3'-C3'	2.08	1.47	1.43
1	C1	2384	OMU	C5-C4	2.07	1.48	1.43
1	C1	627	OMG	C5-C4	-2.05	1.37	1.43
1	C1	1868	OMU	O4-C4	-2.04	1.20	1.24
1	C1	2690	OMU	O4-C4	-2.04	1.20	1.24
1	C1	2384	OMU	O4-C4	-2.03	1.20	1.24
1	C1	2380	OMU	O4-C4	-2.02	1.20	1.24
1	C1	2838	OMC	C4-N3	-2.01	1.30	1.34

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	1847	A2M	C1'-N9-C4	10.82	145.66	126.64
1	C1	389	A2M	C1'-N9-C4	10.53	145.13	126.64
1	C1	1432	A2M	C1'-N9-C4	10.36	144.85	126.64
1	C1	637	A2M	C1'-N9-C4	10.28	144.70	126.64
1	C1	858	A2M	C1'-N9-C4	10.08	144.35	126.64
1	C1	848	A2M	C1'-N9-C4	10.04	144.28	126.64
1	C1	858	A2M	C5-C6-N6	9.78	135.22	120.35
1	C1	1223	A2M	C1'-N9-C4	9.70	143.68	126.64
1	C1	2289	A2M	C1'-N9-C4	9.67	143.62	126.64
1	C1	1223	A2M	C5-C6-N6	9.59	134.92	120.35
1	C1	637	A2M	C5-C6-N6	9.48	134.76	120.35
1	C1	1432	A2M	C5-C6-N6	9.34	134.55	120.35
1	C1	1847	A2M	C5-C6-N6	9.34	134.54	120.35
1	C1	2289	A2M	C5-C6-N6	9.04	134.09	120.35
1	C1	848	A2M	C5-C6-N6	8.98	133.99	120.35
1	C1	389	A2M	C5-C6-N6	8.79	133.71	120.35
1	C1	858	A2M	N6-C6-N1	-6.66	104.75	118.57
1	C1	1847	A2M	N6-C6-N1	-6.50	105.08	118.57
1	C1	1432	A2M	N6-C6-N1	-6.41	105.27	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1223	A2M	N6-C6-N1	-6.36	105.36	118.57
1	C1	637	A2M	N6-C6-N1	-6.27	105.56	118.57
1	C1	848	A2M	N6-C6-N1	-6.17	105.77	118.57
1	C1	2289	A2M	N6-C6-N1	-6.02	106.08	118.57
1	C1	389	A2M	N6-C6-N1	-5.86	106.40	118.57
1	C1	848	A2M	N3-C2-N1	-5.86	119.51	128.68
1	C1	389	A2M	N3-C2-N1	-5.86	119.52	128.68
1	C1	1432	A2M	N3-C2-N1	-5.83	119.56	128.68
1	C1	858	A2M	N3-C2-N1	-5.82	119.58	128.68
1	C1	2289	A2M	N3-C2-N1	-5.82	119.59	128.68
1	C1	1868	OMU	C4-N3-C2	-5.78	118.95	126.58
1	C1	1223	A2M	N3-C2-N1	-5.74	119.70	128.68
1	C1	637	A2M	N3-C2-N1	-5.64	119.86	128.68
1	C1	1847	A2M	N3-C2-N1	-5.56	120.00	128.68
1	C1	2690	OMU	C4-N3-C2	-5.29	119.61	126.58
1	C1	1812	OMC	CM2-O2'-C2'	5.25	128.30	114.52
1	C1	2683	OMU	C4-N3-C2	-5.23	119.69	126.58
1	C1	2380	OMU	C4-N3-C2	-5.13	119.81	126.58
1	C1	2688	OMU	C4-N3-C2	-5.12	119.83	126.58
1	C1	2277	OMU	C4-N3-C2	-5.10	119.85	126.58
1	C1	2384	OMU	C4-N3-C2	-5.09	119.87	126.58
1	C1	1917	OMU	C4-N3-C2	-5.03	119.95	126.58
1	C1	2838	OMC	C1'-N1-C2	4.93	129.41	118.42
1	C1	1868	OMU	N3-C2-N1	4.28	120.57	114.89
1	C1	1917	OMU	N3-C2-N1	4.10	120.34	114.89
1	C1	2690	OMU	N3-C2-N1	3.90	120.07	114.89
1	C1	2380	OMU	N3-C2-N1	3.79	119.92	114.89
1	C1	2277	OMU	N3-C2-N1	3.77	119.90	114.89
1	C1	2683	OMU	C5-C4-N3	3.72	120.41	114.84
1	C1	2384	OMU	N3-C2-N1	3.67	119.77	114.89
1	C1	2688	OMU	N3-C2-N1	3.67	119.77	114.89
1	C1	2838	OMC	C1'-N1-C6	-3.67	112.84	120.84
1	C1	1420	OMC	C1'-N1-C2	3.63	126.53	118.42
1	C1	2683	OMU	N3-C2-N1	3.61	119.68	114.89
1	C1	1868	OMU	C5-C4-N3	3.57	120.18	114.84
1	C1	2380	OMU	C5-C4-N3	3.46	120.01	114.84
1	C1	2384	OMU	C5-C4-N3	3.36	119.86	114.84
1	C1	2688	OMU	C5-C4-N3	3.35	119.86	114.84
1	C1	2690	OMU	C5-C4-N3	3.34	119.84	114.84
1	C1	2277	OMU	C5-C4-N3	3.32	119.81	114.84
1	C1	1917	OMU	C5-C4-N3	3.18	119.59	114.84
1	C1	2683	OMU	O4-C4-C5	-3.05	119.80	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2384	OMU	O4-C4-C5	-3.00	119.89	125.16
1	C1	2838	OMC	O2-C2-N3	-2.95	117.54	122.33
1	C1	1868	OMU	O4-C4-C5	-2.90	120.05	125.16
1	C1	2380	OMU	O4-C4-C5	-2.88	120.10	125.16
1	C1	2690	OMU	O4-C4-C5	-2.87	120.11	125.16
1	C1	2277	OMU	O4-C4-C5	-2.87	120.11	125.16
1	C1	1812	OMC	C2'-C1'-N1	-2.85	108.68	114.22
1	C1	2688	OMU	O4-C4-C5	-2.85	120.15	125.16
1	C1	1917	OMU	C1'-N1-C2	2.75	122.54	117.57
1	C1	2578	OMG	O6-C6-C5	2.68	129.61	124.37
1	C1	627	OMG	O6-C6-C5	2.55	129.35	124.37
1	C1	787	OMG	O6-C6-C5	2.54	129.33	124.37
1	C1	2881	OMG	O6-C6-C5	2.51	129.28	124.37
1	C1	1433	OMG	O6-C6-C5	2.44	129.15	124.37
1	C1	2876	OMG	O6-C6-C5	2.40	129.05	124.37
1	C1	2384	OMU	C1'-N1-C2	2.38	121.88	117.57
1	C1	1917	OMU	O4-C4-C5	-2.38	120.97	125.16
1	C1	1420	OMC	C1'-N1-C6	-2.36	115.69	120.84
1	C1	2774	OMG	O6-C6-C5	2.31	128.89	124.37
1	C1	778	OMC	C1'-N1-C2	2.30	123.56	118.42
1	C1	2380	OMU	O2-C2-N1	-2.29	119.75	122.79
1	C1	2683	OMU	O2-C2-N1	-2.27	119.78	122.79
1	C1	2358	OMG	O6-C6-C5	2.20	128.67	124.37
1	C1	385	OMG	O6-C6-C5	2.18	128.63	124.37
1	C1	2838	OMC	O2-C2-N1	2.17	123.38	118.89
1	C1	1847	A2M	C5'-C4'-C3'	-2.11	107.27	115.18
1	C1	1223	A2M	O4'-C1'-C2'	-2.09	102.96	106.59
1	C1	646	OMG	O6-C6-C5	2.08	128.43	124.37
1	C1	848	A2M	O4'-C1'-C2'	-2.06	103.01	106.59
1	C1	1868	OMU	O2-C2-N1	-2.06	120.05	122.79
1	C1	1420	OMC	O2-C2-N1	2.03	123.08	118.89
1	C1	646	OMG	C5-C6-N1	-2.02	110.38	113.95
1	C1	1917	OMU	O2-C2-N3	-2.00	117.77	121.50

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C1	389	A2M	C1'-C2'-O2'-CM'
1	C1	637	A2M	C1'-C2'-O2'-CM'
1	C1	1433	OMG	O4'-C4'-C5'-O5'
1	C1	1812	OMC	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
1	C1	1847	A2M	C3’-C4’-C5’-O5’
1	C1	1917	OMU	O4’-C4’-C5’-O5’
1	C1	2578	OMG	O4’-C4’-C5’-O5’
1	C1	2683	OMU	C1’-C2’-O2’-CM2
1	C1	2690	OMU	C3’-C4’-C5’-O5’
1	C1	2690	OMU	O4’-C4’-C5’-O5’
1	C1	2838	OMC	O4’-C1’-N1-C2
1	C1	2838	OMC	O4’-C1’-N1-C6
1	C1	389	A2M	O4’-C4’-C5’-O5’
1	C1	1433	OMG	C3’-C4’-C5’-O5’
1	C1	1847	A2M	O4’-C4’-C5’-O5’
1	C1	1917	OMU	C3’-C4’-C5’-O5’
1	C1	2578	OMG	C3’-C4’-C5’-O5’
1	C1	1812	OMC	C3’-C2’-O2’-CM2
1	C1	385	OMG	C3’-C4’-C5’-O5’
1	C1	389	A2M	C3’-C4’-C5’-O5’
1	C1	385	OMG	O4’-C4’-C5’-O5’
1	C1	2300	OMC	C1’-C2’-O2’-CM2
1	C1	2578	OMG	C4’-C5’-O5’-P
1	C1	1420	OMC	C3’-C2’-O2’-CM2
1	C1	1847	A2M	C4’-C5’-O5’-P
1	C1	1420	OMC	C2’-C1’-N1-C6
1	C1	1223	A2M	O4’-C4’-C5’-O5’
1	C1	1433	OMG	C1’-C2’-O2’-CM2
1	C1	1420	OMC	C2’-C1’-N1-C2
1	C1	1491	OMC	O4’-C4’-C5’-O5’
1	C1	1420	OMC	O4’-C4’-C5’-O5’

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	**Type**	**Chain**	**Res**	**Link**	**Bond lengths**			**Bond angles**		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	GTP	Cd	1000	60	26,34,34	1.22	1 (3%)	32,54,54	1.49	7 (21%)
59	GTP	CH	701	60	26,34,34	1.22	1 (3%)	32,54,54	1.48	7 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	**Type**	**Chain**	**Res**	**Link**	**Chirals**	**Torsions**	**Rings**
59	GTP	Cd	1000	60	-	3/18/38/38	0/3/3/3
59	GTP	CH	701	60	-	6/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Atoms**	**Z**	**Observed(Å)**	**Ideal(Å)**
59	CH	701	GTP	C5-C6	-4.35	1.38	1.47
59	Cd	1000	GTP	C5-C6	-4.30	1.38	1.47

All (14) bond angle outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Atoms**	**Z**	**Observed(^{o})**	**Ideal(^{o})**
59	Cd	1000	GTP	PB-O3B-PG	-3.35	121.33	132.83
59	CH	701	GTP	C5-C6-N1	3.15	119.52	113.95
59	Cd	1000	GTP	C5-C6-N1	3.11	119.45	113.95
59	CH	701	GTP	O2G-PG-O3B	3.10	115.02	104.64
59	CH	701	GTP	C8-N7-C5	3.03	108.77	102.99
59	Cd	1000	GTP	C8-N7-C5	3.02	108.74	102.99
59	CH	701	GTP	C2-N1-C6	-2.85	119.84	125.10
59	CH	701	GTP	PB-O3B-PG	-2.77	123.32	132.83
59	Cd	1000	GTP	C2-N1-C6	-2.66	120.19	125.10
59	CH	701	GTP	PA-O3A-PB	-2.64	123.77	132.83
59	Cd	1000	GTP	PA-O3A-PB	-2.32	124.88	132.83
59	CH	701	GTP	O6-C6-C5	-2.16	120.16	124.37
59	Cd	1000	GTP	O3G-PG-O3B	2.12	111.73	104.64
59	Cd	1000	GTP	O6-C6-C5	-2.02	120.42	124.37

There are no chirality outliers.

All (9) torsion outliers are listed below:

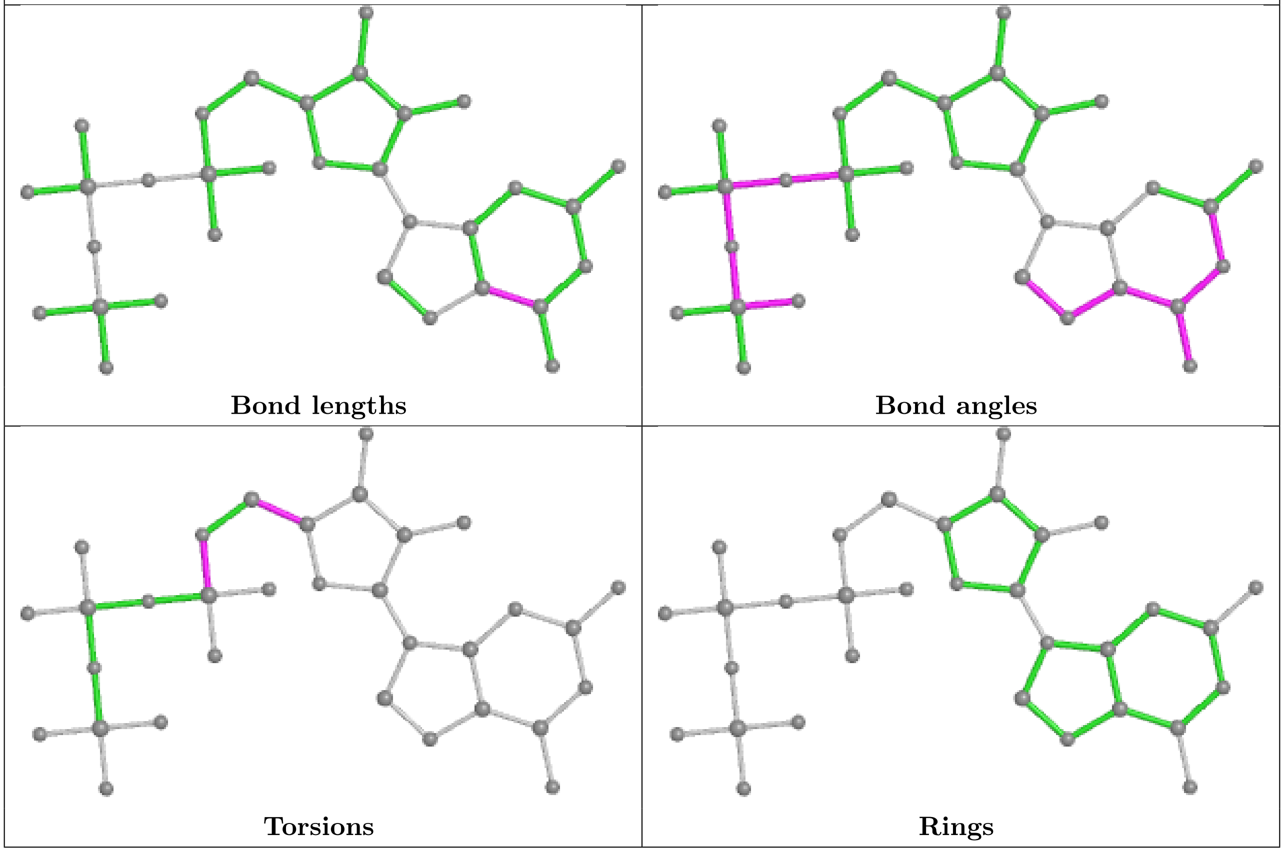
Mol	Chain	Res	Type	Atoms
59	CH	701	GTP	C5'-O5'-PA-O3A
59	CH	701	GTP	O4'-C4'-C5'-O5'
59	CH	701	GTP	C3'-C4'-C5'-O5'
59	CH	701	GTP	C5'-O5'-PA-O1A
59	CH	701	GTP	C5'-O5'-PA-O2A
59	Cd	1000	GTP	O4'-C4'-C5'-O5'
59	Cd	1000	GTP	C3'-C4'-C5'-O5'
59	CH	701	GTP	PB-O3A-PA-O2A
59	Cd	1000	GTP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GTP Cd 1000



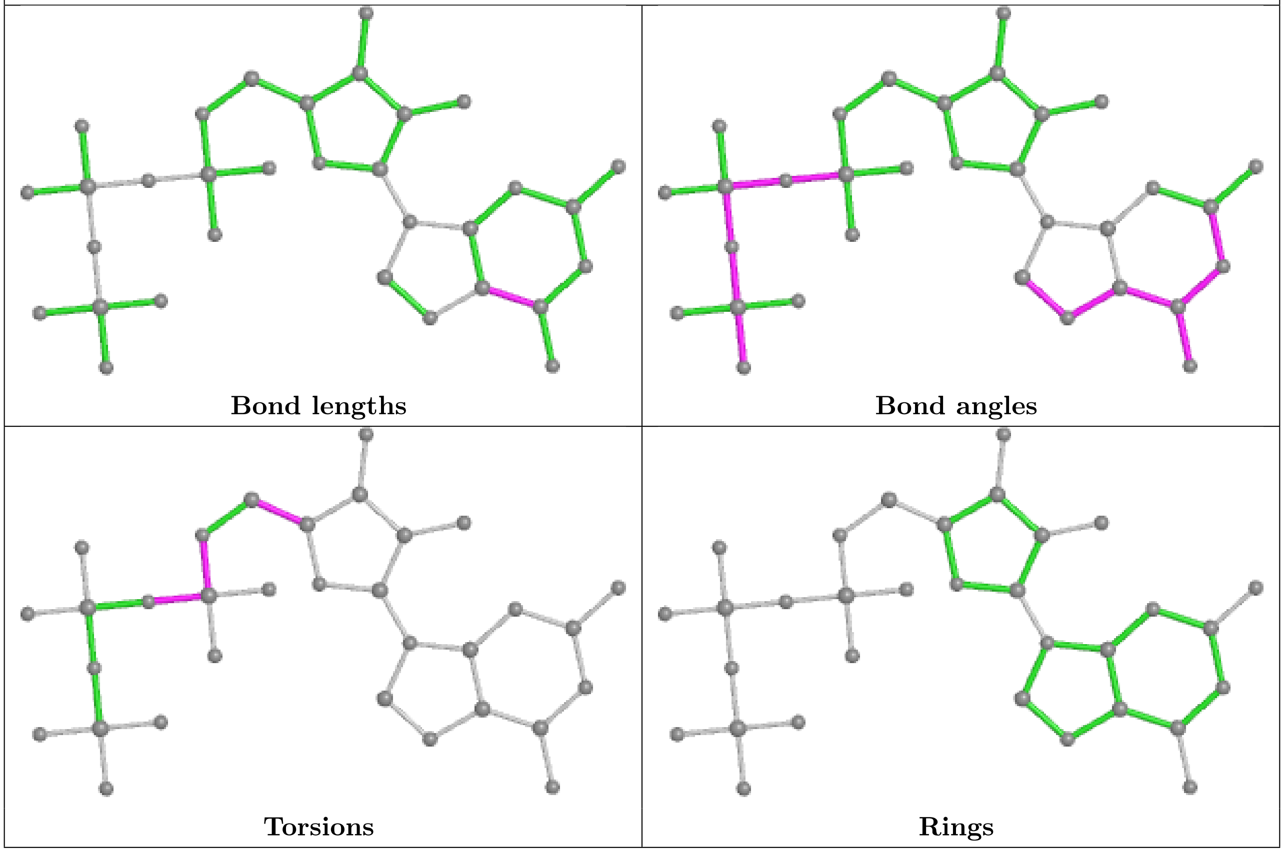
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP CH 701



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

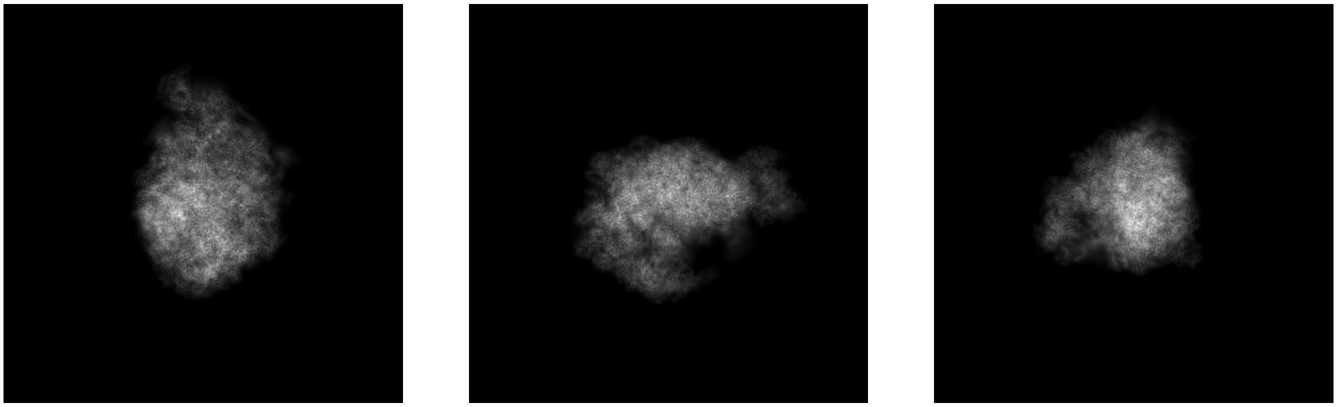
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-17956. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

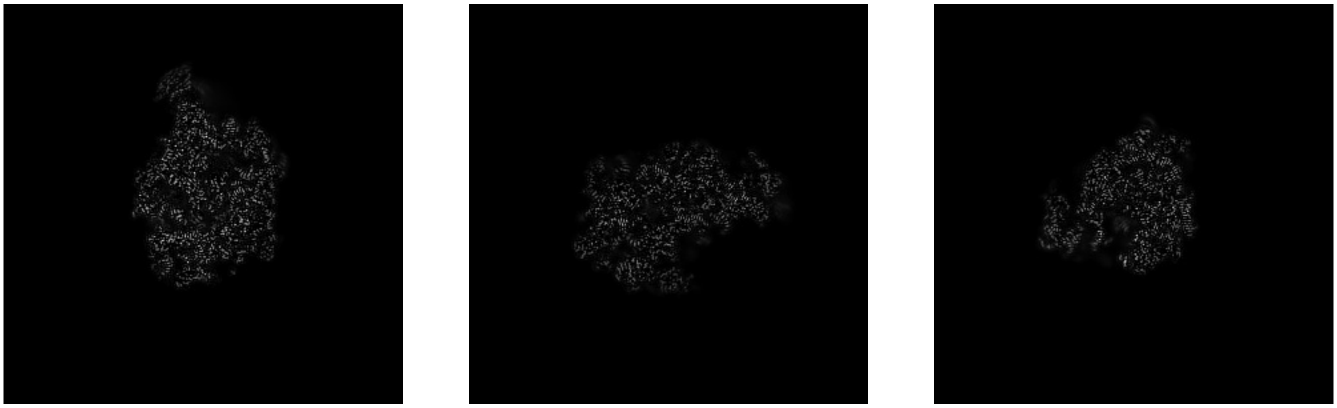


X Y Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map

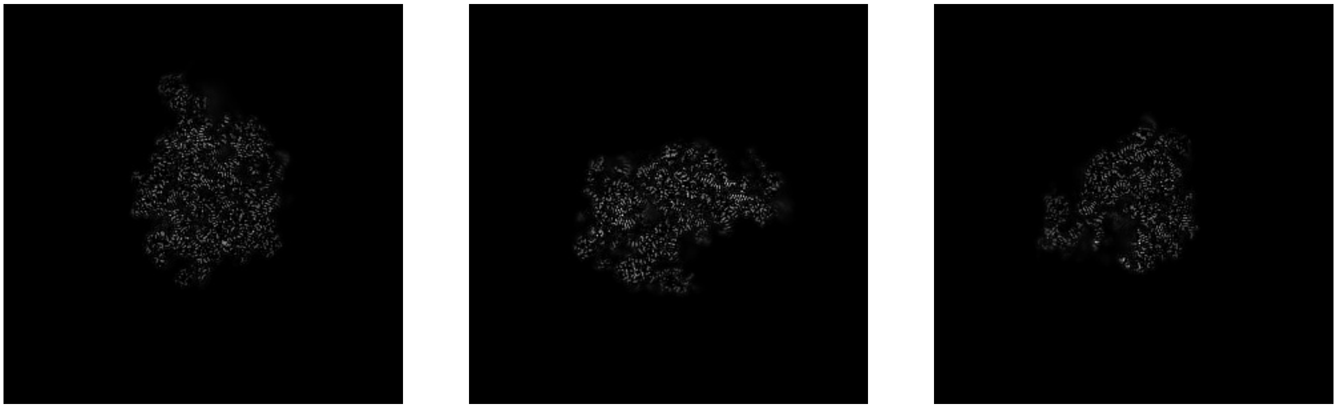


X Index: 250 Y Index: 250 Z Index: 250

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

6.3.1 Primary map

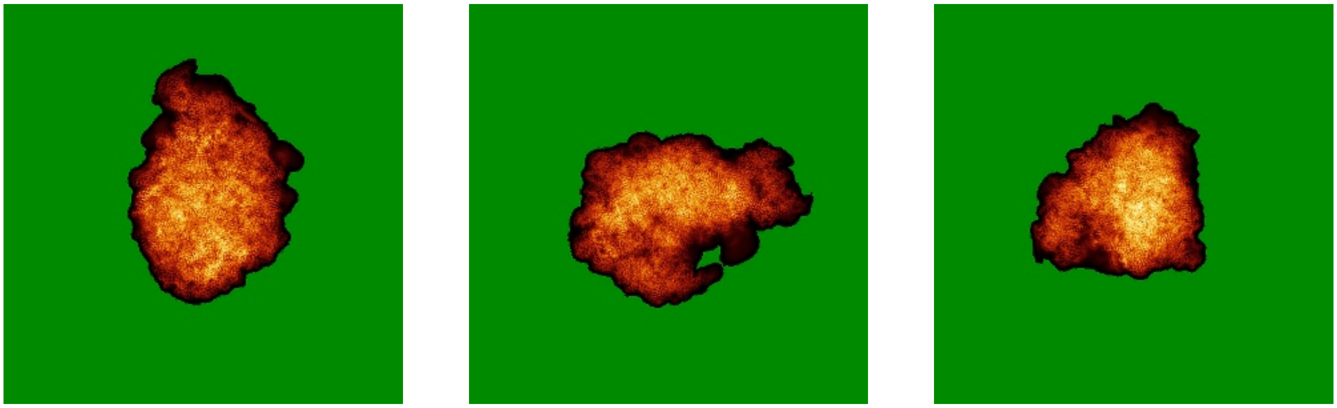


X Index: 259 Y Index: 248 Z Index: 252

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



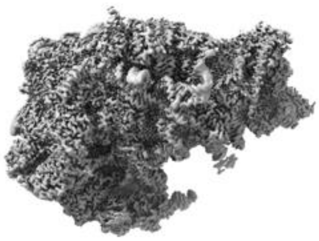
X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

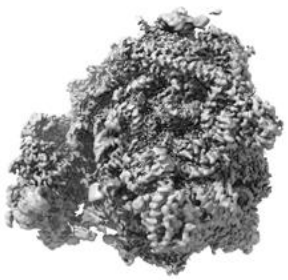
6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

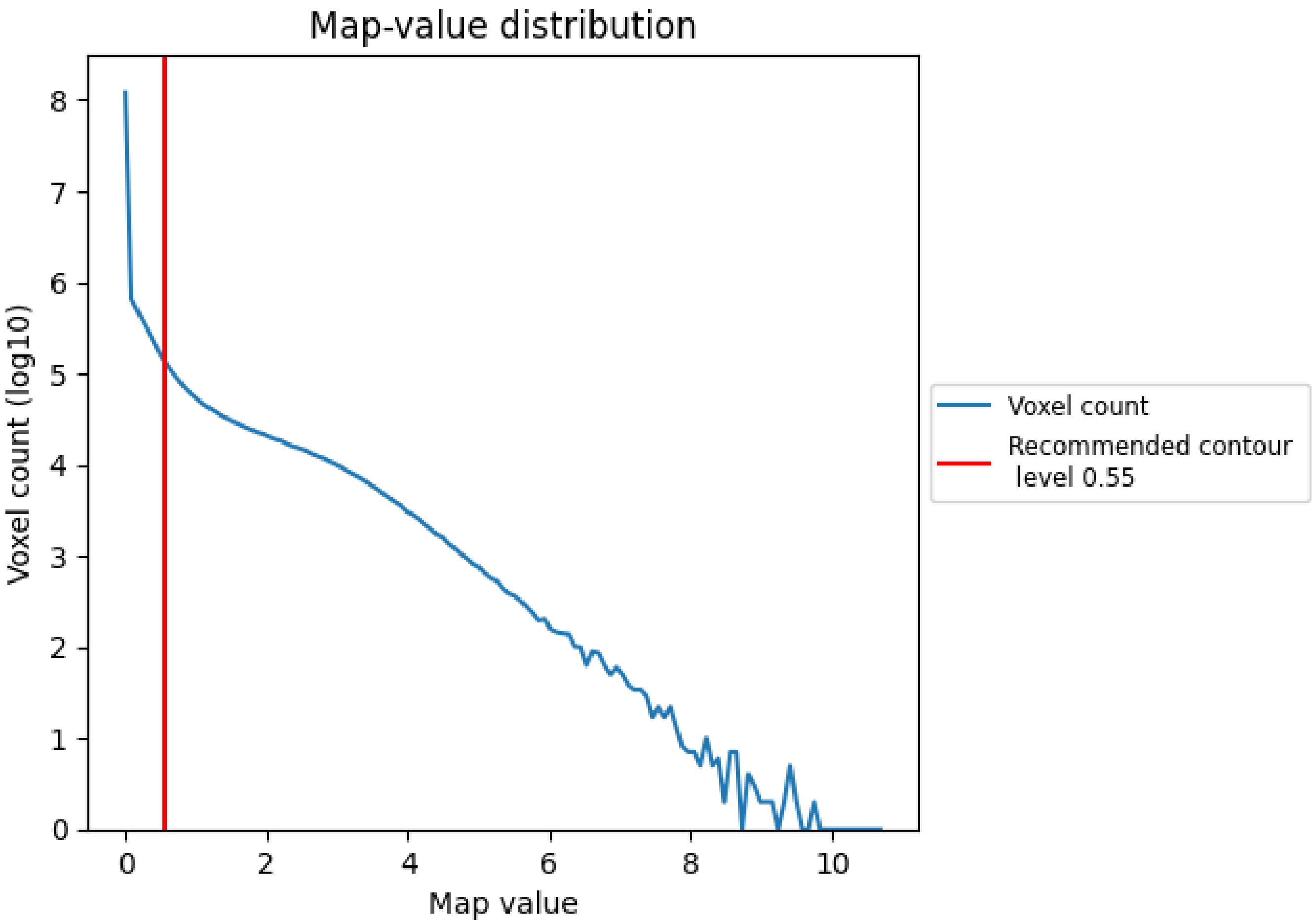
6.6 Mask visualisation ⓘ

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

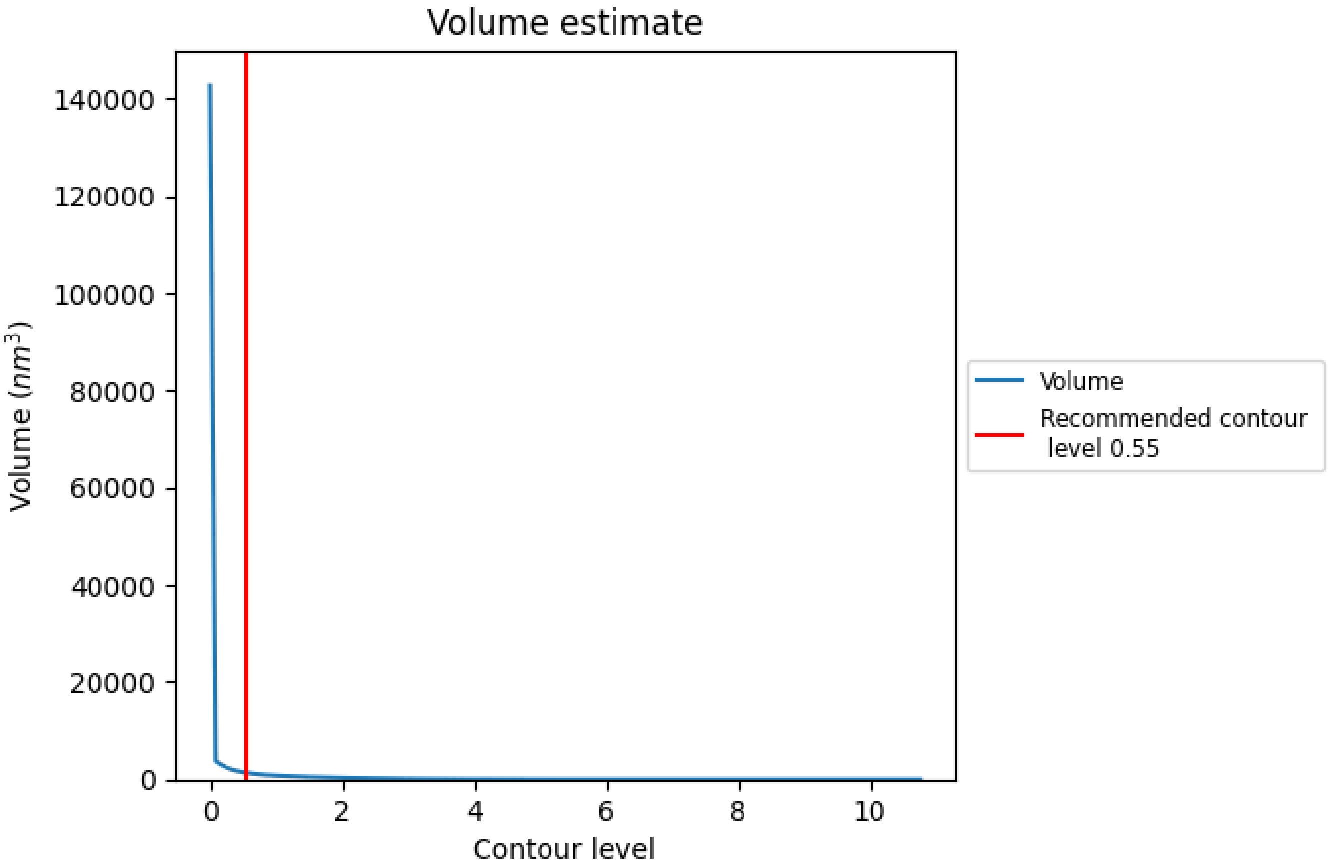
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

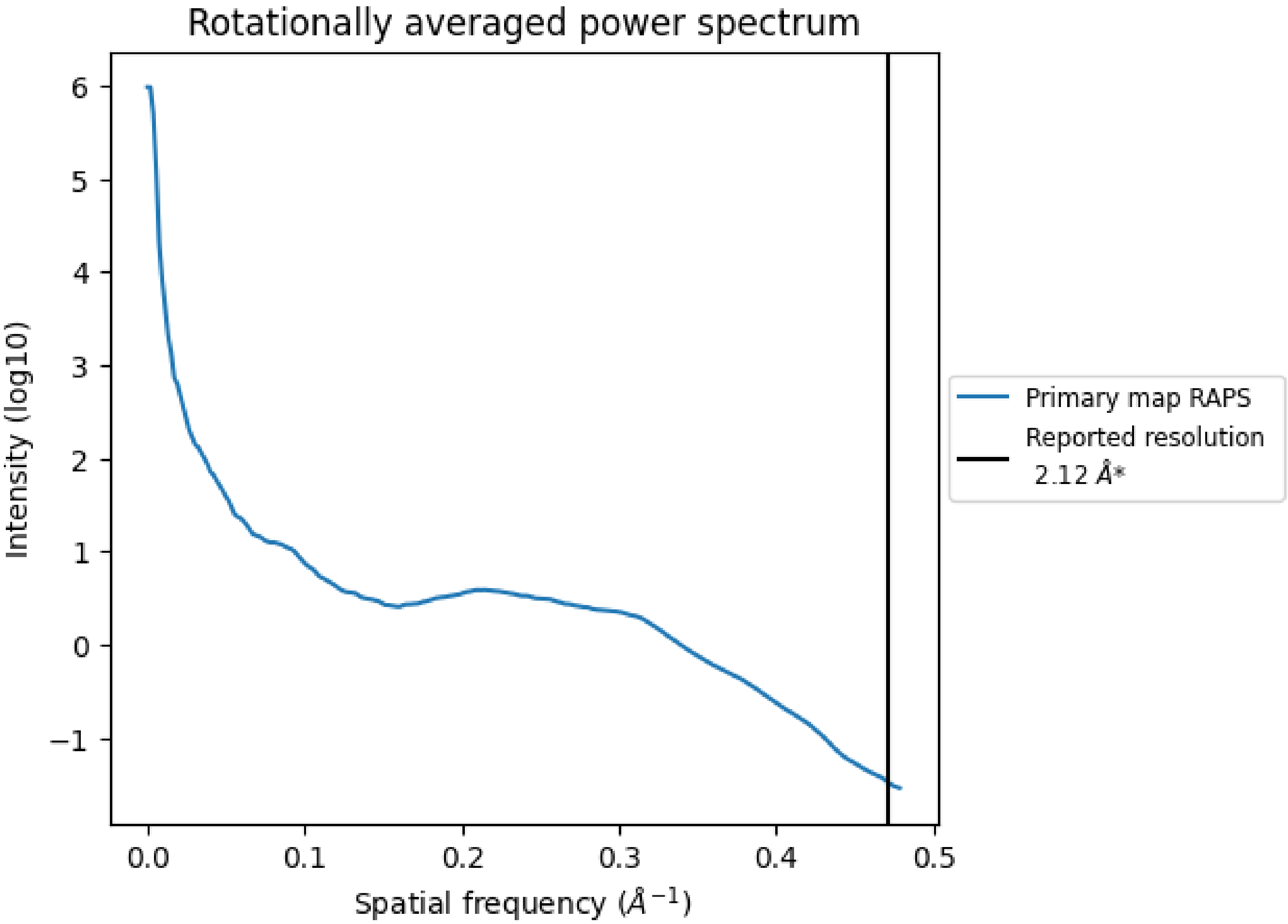
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1355 nm^3; this corresponds to an approximate mass of 1224 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.472 $Å^{-1}$

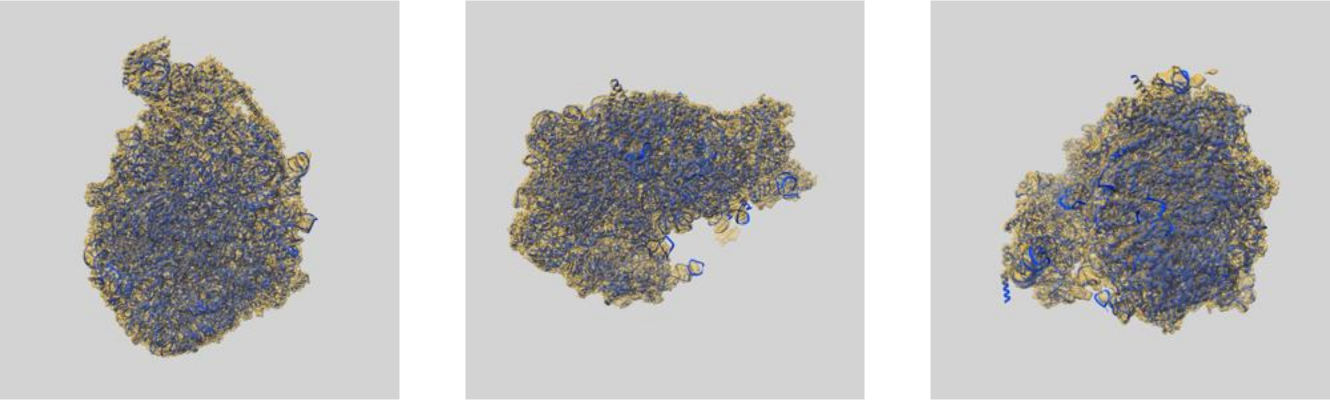
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-17956 and PDB model 8PV7. Per-residue inclusion information can be found in section 3 on page 16.

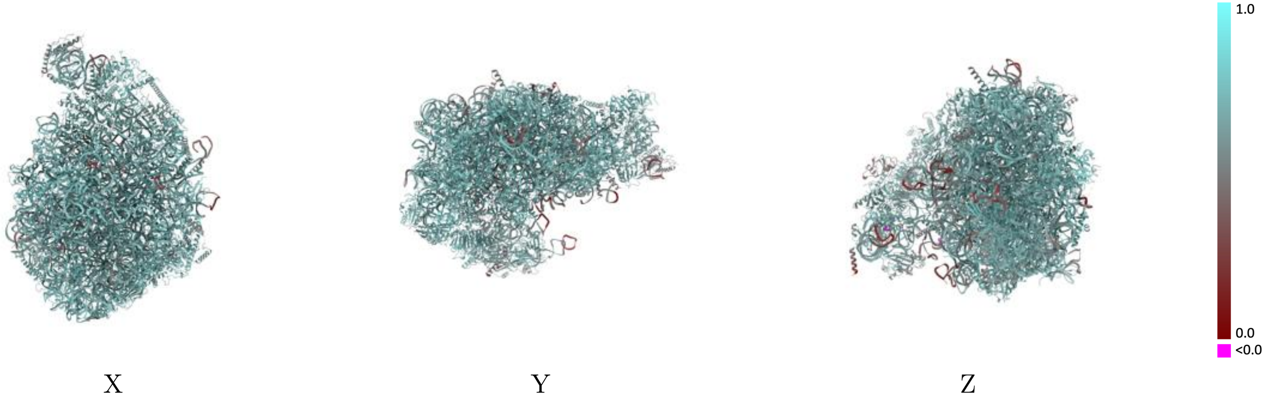
9.1 Map-model overlay ⓘ



X Y Z

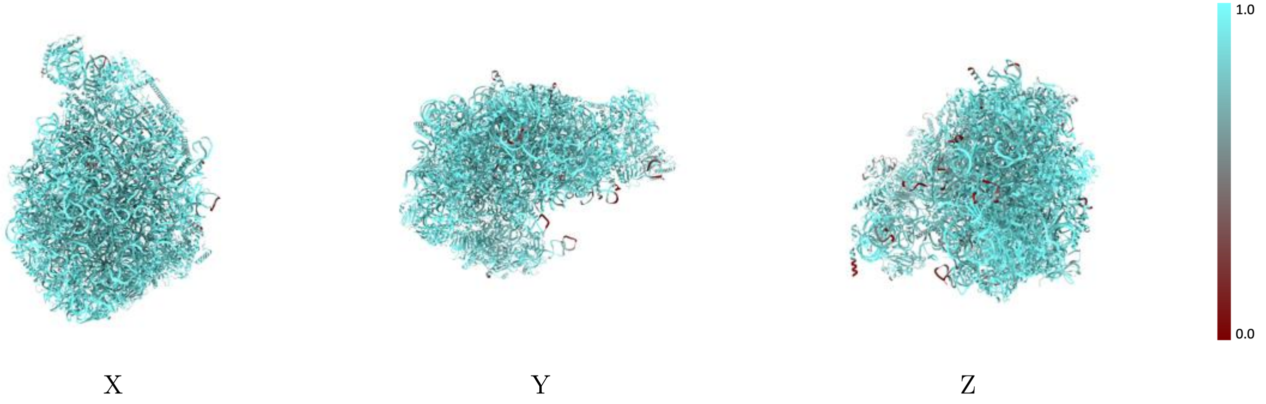
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



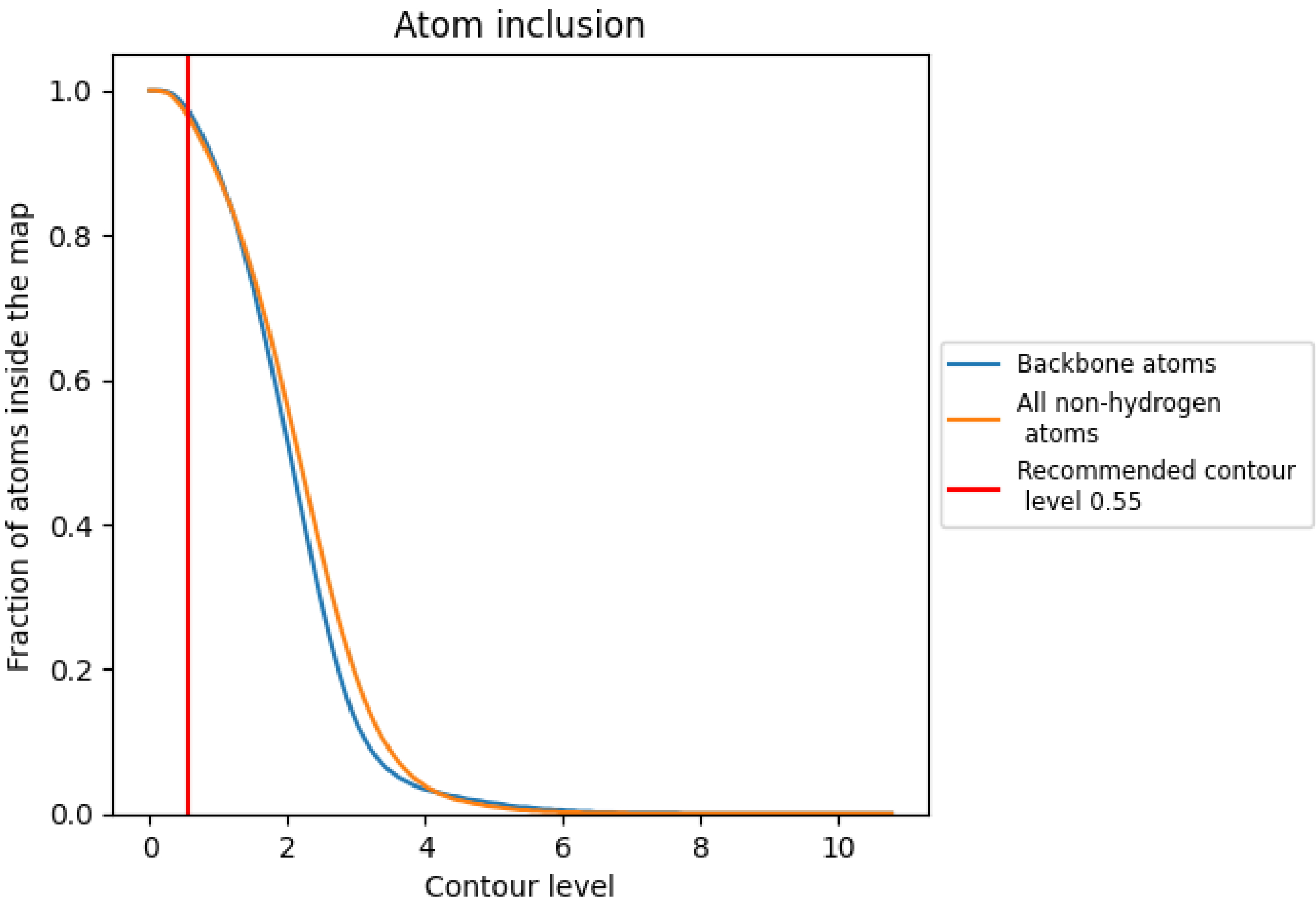
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.55).

9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9650	0.6760
C1	0.9770	0.6650
C2	0.9770	0.6890
C3	0.8300	0.5370
C4	0.9280	0.5990
CB	0.9290	0.6250
CF	0.9670	0.6860
CH	0.9490	0.6920
CI	0.9200	0.6380
CJ	0.9840	0.6940
CK	0.9860	0.7230
CL	0.9440	0.6420
CM	0.9520	0.6590
CN	0.9730	0.7110
CO	0.9520	0.7060
CQ	0.9210	0.6770
Cb	0.9750	0.7070
Cd	0.9690	0.7000
Ce	0.8940	0.6380
Cf	0.9640	0.6740
Cg	0.9650	0.6590
Ch	0.9210	0.6570
Cz	0.8810	0.5970
LA	0.9870	0.7100
LB	0.9850	0.7300
LC	0.9810	0.7230
LD	0.9300	0.6620
LE	0.9440	0.6810
LF	0.9770	0.7050
LG	0.9720	0.6990
LH	0.9730	0.7150
LJ	0.9290	0.5920
LK	0.9410	0.6470
LL	0.9610	0.7030
LM	0.9730	0.7060

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Chain	Atom inclusion	Q-score
LN	0.9960	0.7310
LO	0.9890	0.7290
LP	0.9870	0.7210
LQ	0.9860	0.7000
LR	0.9620	0.7080
LS	0.9880	0.7080
LT	0.9490	0.6280
LU	0.9410	0.6620
LV	0.9910	0.7310
LX	0.9730	0.6940
LY	0.9770	0.7080
LZ	0.9670	0.7020
La	0.9730	0.7060
Lc	0.9600	0.6890
Ld	0.9660	0.7160
Le	0.9880	0.7310
Lf	0.9960	0.7380
Lg	0.9340	0.6940
Lh	0.9460	0.6620
Li	0.9500	0.6780
Lj	0.9930	0.7380
Lk	0.9170	0.6740
Ll	0.9980	0.7390
Lp	0.9480	0.6910
Lq	0.9690	0.6970